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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	3	OCT 19	BEILSTEIN updated with new compounds
NEWS	4	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	5	NOV 19	WPIX enhanced with XML display format
NEWS	6	NOV 30	ICSD reloaded with enhancements
NEWS	7	DEC 04	LINPADOCDB now available on STN
NEWS	8	DEC 14	BEILSTEIN pricing structure to change
NEWS	9	DEC 17	USPATOLD added to additional database clusters
NEWS	10	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	11	DEC 17	DGENE now includes more than 10 million sequences
NEWS	12	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	13	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS	14	DEC 17	CA/CAPplus enhanced with new custom IPC display formats
NEWS	15	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	16	JAN 02	STN pricing information for 2008 now available
NEWS	17	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	18	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	19	JAN 28	MARPAT searching enhanced
NEWS	20	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	21	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	22	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	23	FEB 08	STN Express, Version 8.3, now available
NEWS	24	FEB 20	PCI now available as a replacement to DPCI
NEWS	25	FEB 25	IFIREF reloaded with enhancements
NEWS	26	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	27	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:43:49 ON 11 MAR 2008

=> file registry

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:44:13 ON 11 MAR 2008

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STRUCTURE FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

DICTIONARY FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

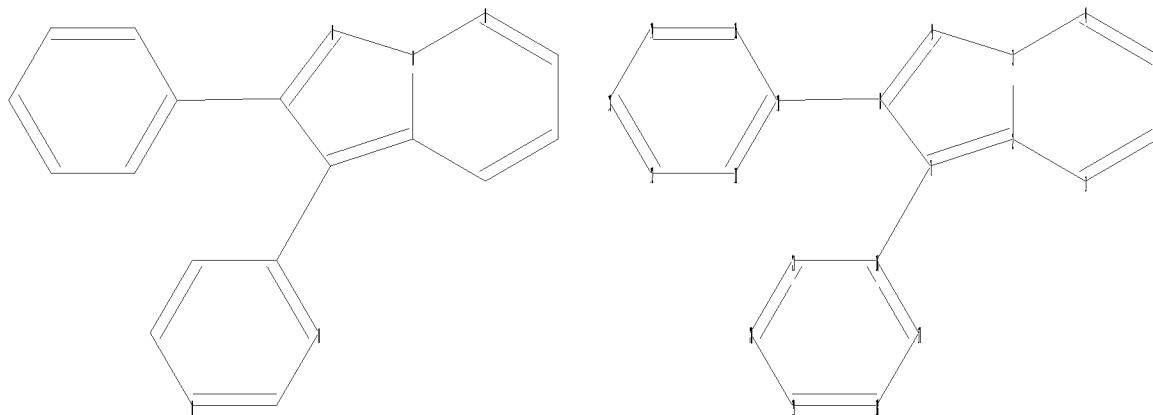
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10 series\10530985\10530985b.str



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21

chain bonds :

7-16 8-10

```

ring bonds :
1-2  1-6  2-3  2-7  3-4  3-9  4-5  5-6  7-8  8-9  10-11  10-15  11-12  12-13  13-14
 14-15 16-17 16-21 17-18 18-19 19-20 20-21
exact/norm bonds :
1-2  1-6  2-3  2-7  3-4  3-9  4-5  5-6  7-8  8-9
exact bonds :
7-16  8-10
normalized bonds :
10-11  10-15  11-12  12-13  13-14  14-15  16-17  16-21  17-18  18-19  19-20  20-21

```

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Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom

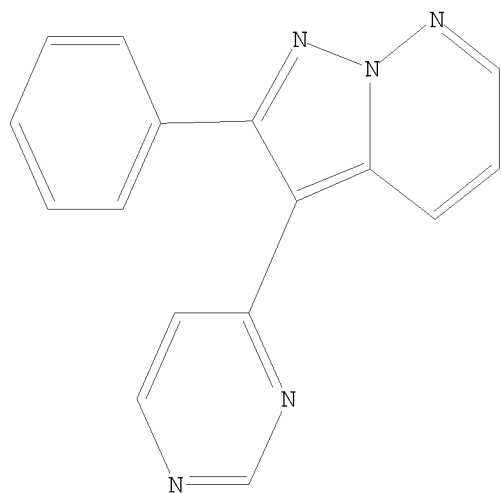
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L1 STRUCTURE UPLOADED

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=> d l1
L1 HAS NO ANSWERS
L1            STR

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Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 10:44:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -            0 TO ITERATE

100.0% PROCESSED            0 ITERATIONS            0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                         BATCH  **COMPLETE**
PROJECTED ITERATIONS:            0 TO            0
PROJECTED ANSWERS:               0 TO            0

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L2 0 SEA SSS SAM L1

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=> s l1 full

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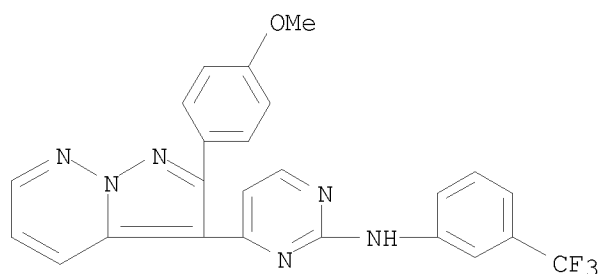
FULL SEARCH INITIATED 10:44:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 95 TO ITERATE

100.0% PROCESSED 95 ITERATIONS 50 ANSWERS
SEARCH TIME: 00.00.01

L3 50 SEA SSS FUL L1

=> d scan

L3 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Pyrimidinamine, 4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-
[3-(trifluoromethyl)phenyl]-
MF C24 H17 F3 N6 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	178.36	178.57

FILE 'CAPLUS' ENTERED AT 10:44:54 ON 11 MAR 2008
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FILE LAST UPDATED: 10 Mar 2008 (20080310/ED)

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<http://www.cas.org/infopolicy.html>

=> s 13

L4 6 L3

=> d 14 1-6 ibib abs hitstr

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:808556 CAPLUS

DOCUMENT NUMBER: 148:208751

TITLE: Construction of the pharmacophore model of glycogen synthase kinase-3 inhibitors

AUTHOR(S): Liu, Ling; Zhang, Li-Na; Jiang, Feng-Chao

CORPORATE SOURCE: School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan, Hubei, 430030, Peop. Rep. China

SOURCE: Chinese Journal of Chemistry (2007), 25(7), 892-897

CODEN: CJOCEV; ISSN: 1001-604X

PUBLISHER: Shanghai Institute of Organic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A three dimensional pharmacophore model has been generated for glycogen synthase kinase-3 (GSK-3) inhibitors. A dataset consisting of 89 compds. was selected on the basis of the information content of the structures and activity data as required by the CATALYST system. The optimum model with four features (one hydrogen-bond acceptor unit, one ring aromatic unit, and two hydrophobic aromatic units) was selected with a good correlation coefficient

(0.95). This model is able to predict the activity of other known GSK-3 inhibitors not included in the model generation, and can be further used to identify structurally diverse compds. with desired biol. activity by virtual screening.

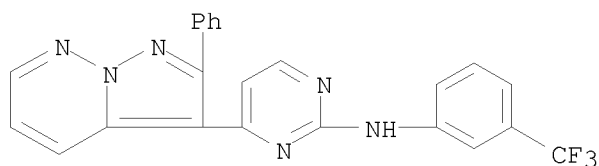
IT 681432-52-0 681432-53-1 681432-55-3
681432-60-0 681432-61-1 681432-62-2
681432-63-3 681432-67-7 681432-71-3
681432-74-6 681432-75-7 681432-76-8
681432-77-9 681432-85-9 681432-88-2
681432-89-3 681432-90-6

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmacophore model of glycogen synthase kinase-3 inhibitors)

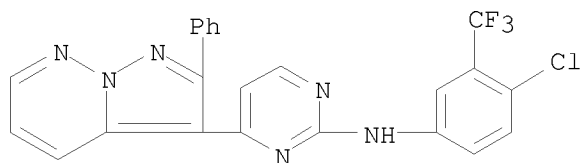
RN 681432-52-0 CAPLUS

CN 2-Pyrimidinamine, 4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



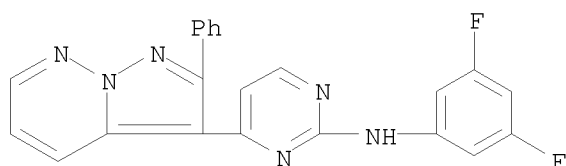
RN 681432-53-1 CAPLUS

CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



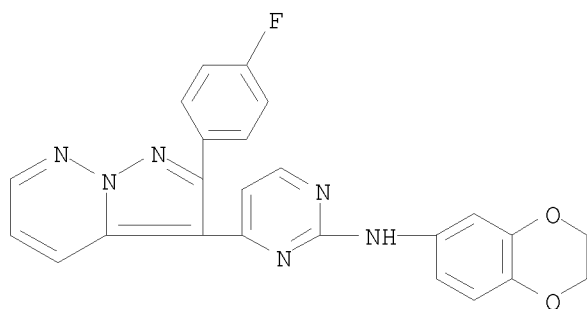
RN 681432-55-3 CAPLUS

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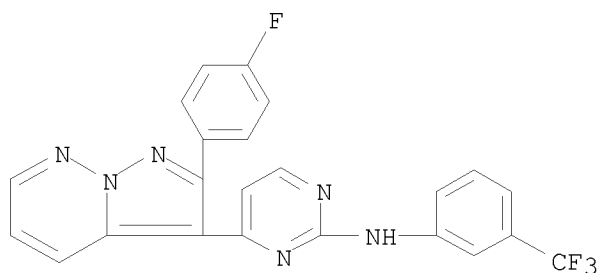
RN 681432-60-0 CAPLUS

CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



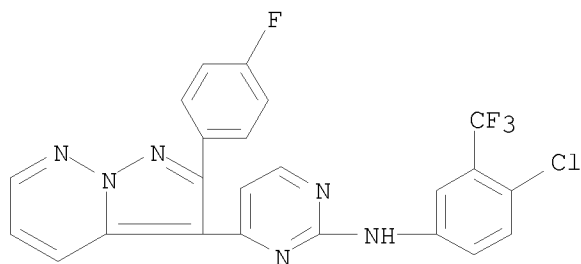
RN 681432-61-1 CAPLUS

CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



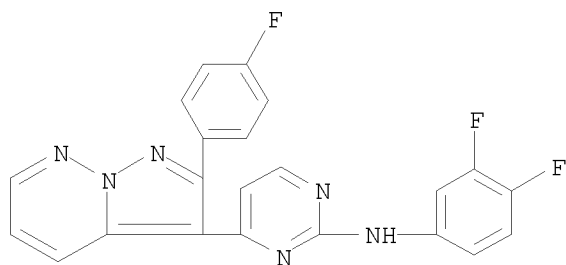
RN 681432-62-2 CAPLUS

CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



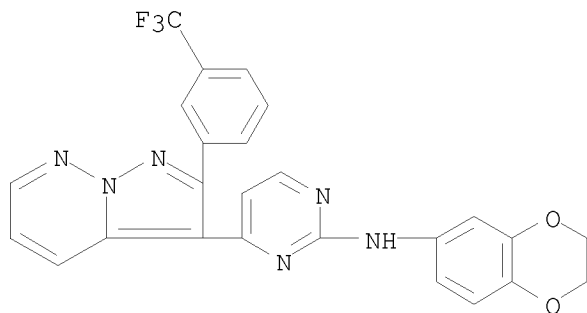
RN 681432-63-3 CAPLUS

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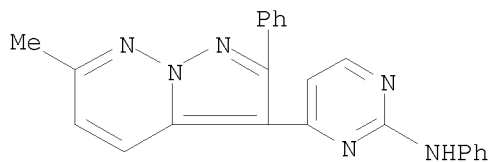
RN 681432-67-7 CAPLUS

CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



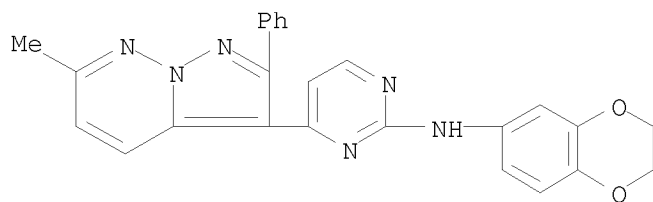
RN 681432-71-3 CAPLUS

CN 2-Pyrimidinamine, 4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-phenyl- (CA INDEX NAME)



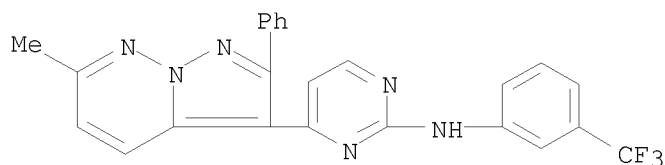
RN 681432-74-6 CAPLUS

CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



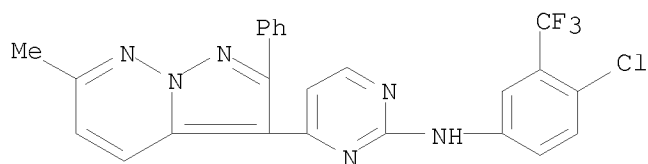
RN 681432-75-7 CAPLUS

CN 2-Pyrimidinamine, 4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



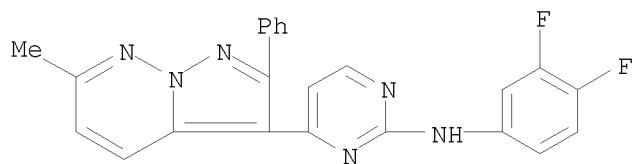
RN 681432-76-8 CAPLUS

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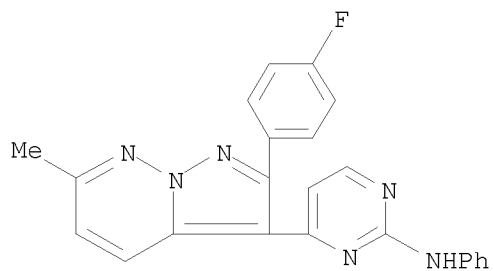
RN 681432-77-9 CAPLUS

CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)

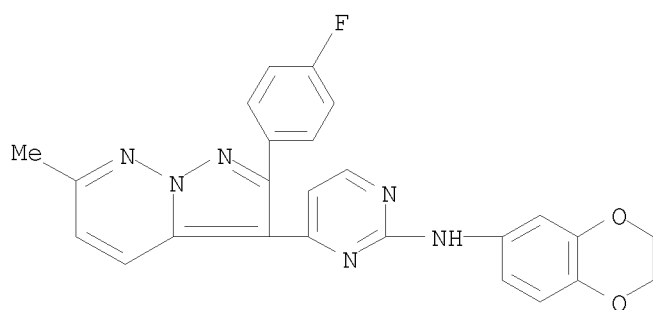


RN 681432-85-9 CAPLUS

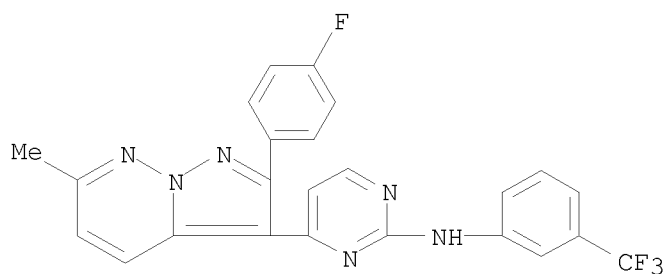
CN 2-Pyrimidinamine, 4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl- (CA INDEX NAME)



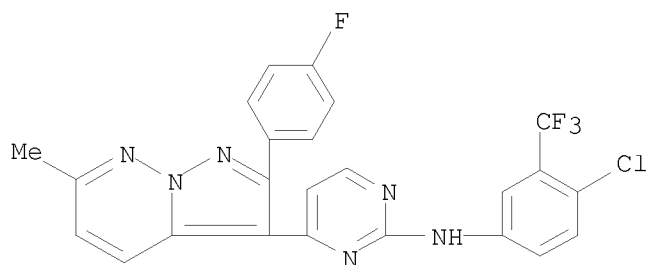
RN 681432-88-2 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



RN 681432-89-3 CAPLUS
 CN 2-Pyrimidinamine, 4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 681432-90-6 CAPLUS
 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:634999 CAPLUS

DOCUMENT NUMBER: 145:103711

TITLE: Preparation of 2-pyrimidinyl pyrazolopyridines as ErbB kinase inhibitors for treating neoplasm

INVENTOR(S): Uehling, David Edward; Stevens, Kirk Lawrence; Dickerson, Scott Howard; Waterson, Alex Gregory; Harris, Philip Anthony; Sammond, Douglas McCord; Hubbard, Robert Dale; Emerson, Holly Kathleen; Wilson, Joseph W.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 255 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

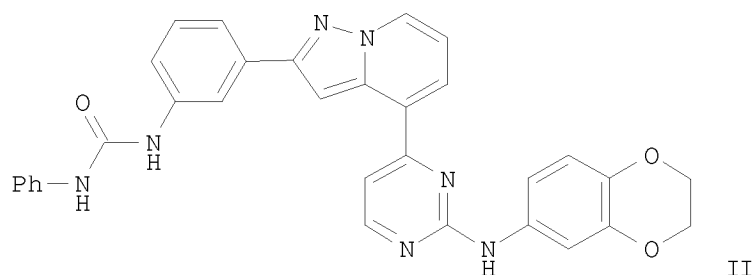
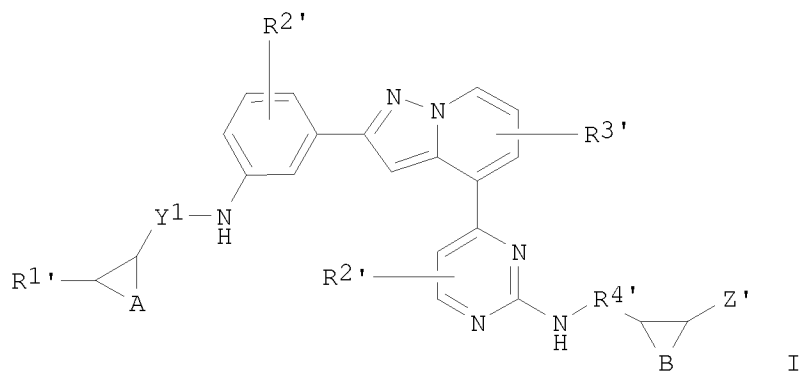
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006068826	A2	20060629	WO 2005-US44166	20051206
WO 2006068826	A3	20061005		
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RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
EP 1828185	A2	20070905	EP 2005-853157	20051206
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR			
US 2008051395	A1	20080228	US 2007-721504	20070612
PRIORITY APPLN. INFO.:			US 2004-637928P	P 20041221
			US 2005-709079P	P 20050817
			WO 2005-US44166	W 20051206

OTHER SOURCE(S): MARPAT 145:103711

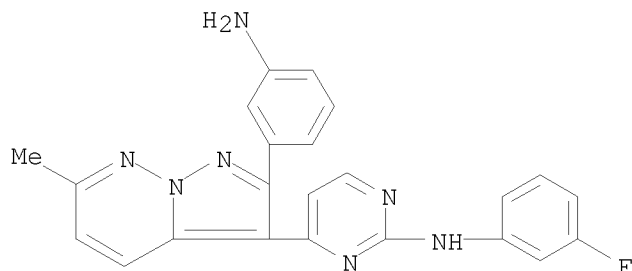
GI



AB Title compds. I [R1' = (R1)a; a = 0-3; each R1 = independently alk(en/yn)yl, (un)substituted hetero/aryl, etc.; A = hetero/aryl, heterocyclyl; Y1 = CO, NHCO, CS, NHCS; R2' = (R2)b; each b = independently 0-2; each R2 = independently halo, alkyl, CN, NO2, etc.; R3' = (R3)d; d = 0-2; each R3 = independently halo, alk(en/yn)yl, aryloxy, arylaminocarbonyl, etc.; R4' = (R4)e; e = 0-1; each R4 = independently alk(en)ylene; B = hetero/aryl; Z' = (Z)g; g = 0-4; Z = (Alk)m-(Y2)n-(Alk)p-(R5)q; m, n, p = independently 0-1; each Alk = independently alk(en)ylene; Y2 = O, CO, SO, NH, etc.; R5 = independently CN, NO2, halo, aryloxy, NH2 and derivs., etc.; and their pharmaceutically acceptable salts, and solvates] were prepared as ErbB kinase inhibitors for treating cancer. Thus, cyclization of 2-(methylthio)-4-[(3-nitrophenyl)ethynyl]pyrimidine (preparation given) with 1-aminopyridinium iodide, oxidation, reaction of sulfoxide with 1,4-benzodioxan-6-amine, reduction

of the nitro intermediate gave pyrazolopyridine, and reaction of the amine with Ph isocyanate gave pyrimidine II. Selected I showed inhibitory activity vs. EGFR or ErbB-2 protein tyrosine kinases with a pIC50 ≥ 7. Selected I showed antiproliferative activity of less than 100 nM in at least one of BT474, HN5 and Colo205 tumor cell lines. I are useful in the treatment of diseases associated with inappropriate ErbB family kinase activity.

IT 895635-94-6, 4-[2-(3-Aminophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-(3-fluorophenyl)-2-pyrimidinamine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 2-pyrimidinyl pyrazolopyridines as ErbB kinase inhibitors for treating neoplasm)
 RN 895635-94-6 CAPLUS
 CN 2-Pyrimidinamine, 4-[2-(3-aminophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-(3-fluorophenyl)- (CA INDEX NAME)



L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:517586 CAPLUS

DOCUMENT NUMBER: 145:76028

TITLE: QSAR modeling of the inhibition of Glycogen Synthase Kinase-3

AUTHOR(S): Katritzky, Alan R.; Pacureanu, Liliana M.; Dobchev, Dimitar A.; Fara, Dan C.; Duchowicz, Pablo R.; Karelson, Mati

CORPORATE SOURCE: Center for Heterocyclic Compounds, Department of Chemistry, University of Florida, Gainesville, FL, 32611, USA

SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(14), 4987-5002

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

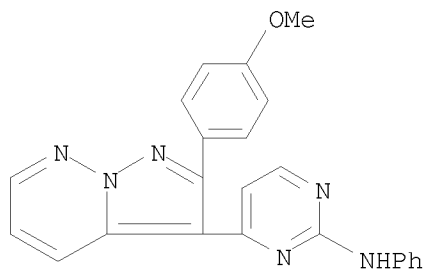
AB Quant. structure-activity relationship (QSAR) models of the biol. activity (pIC50) of 277 inhibitors of Glycogen Synthase Kinase-3 (GSK-3) are developed using geometrical, topol., quantum mech., and electronic descriptors calculated by CODESSA PRO. The linear (multilinear regression) and nonlinear (artificial neural network) models obtained link the structures to their reported activity pIC50. The results are discussed in the light of the main factors that influence the inhibitory activity of the GSK-3 enzyme.

IT 681432-02-0 681432-05-3 681432-06-4
681432-07-5 681432-10-0 681432-20-2
681432-23-5 681432-24-6 681432-25-7
681432-26-8 681432-49-5 681432-52-0
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681432-82-6 681432-83-7 681432-84-8
681432-85-9 681432-88-2 681432-89-3
681432-90-6 681432-91-7

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR modeling of glycogen synthase kinase-3 inhibition)

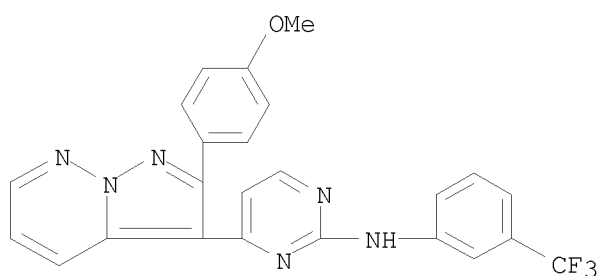
RN 681432-02-0 CAPLUS

CN 2-Pyrimidinamine, 4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl- (CA INDEX NAME)



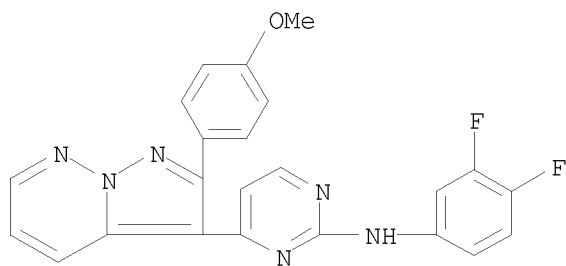
RN 681432-05-3 CAPLUS

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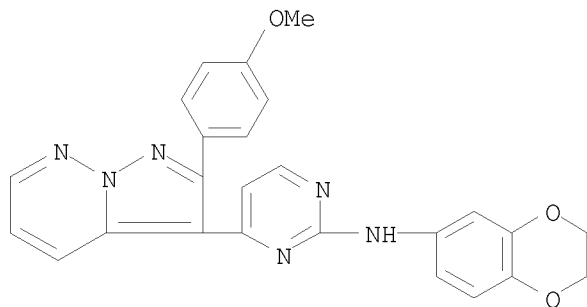
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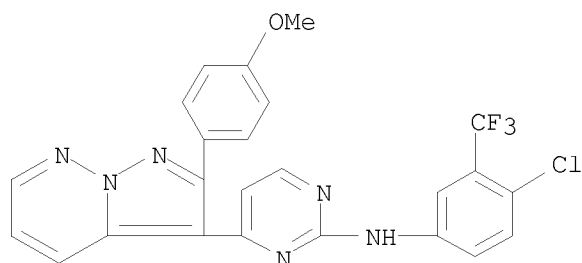


RN 681432-07-5 CAPLUS

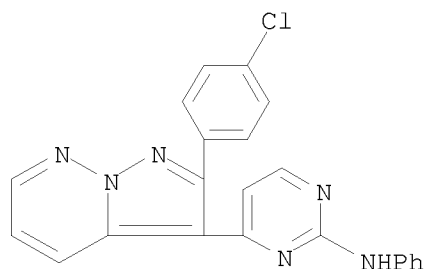
CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



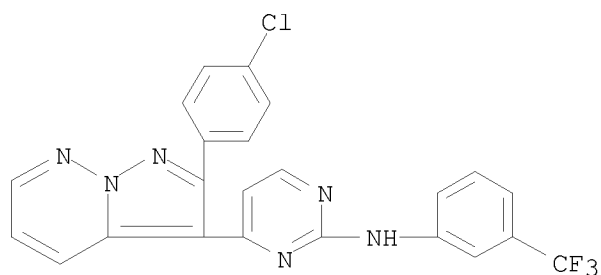
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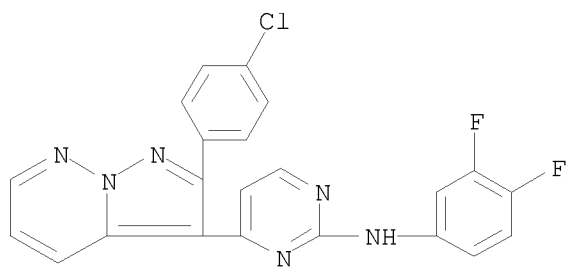
RN 681432-20-2 CAPLUS
 CN 2-Pyrimidinamine, 4-[2-(4-chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl- (CA INDEX NAME)



RN 681432-23-5 CAPLUS
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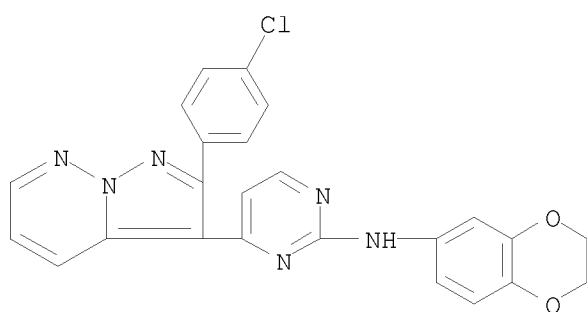


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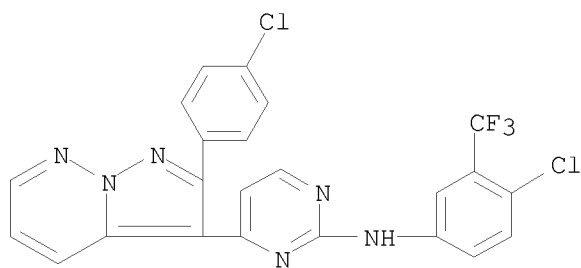
RN 681432-25-7 CAPLUS

CN 2-Pyrimidinamine, 4-[2-(4-chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-(2,3-dihydro-1,4-benzodioxin-6-yl)- (CA INDEX NAME)



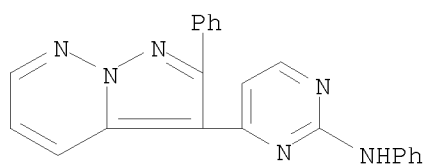
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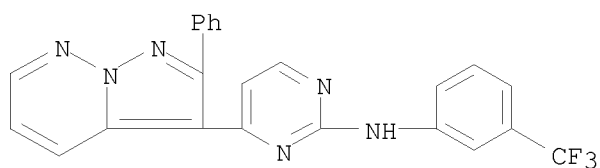
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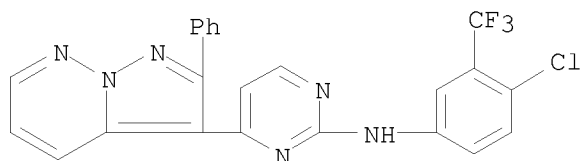
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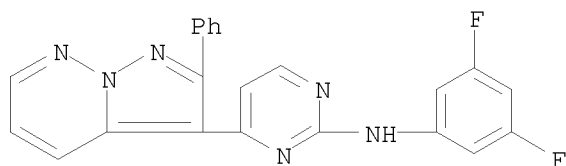
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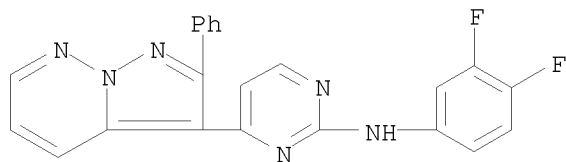
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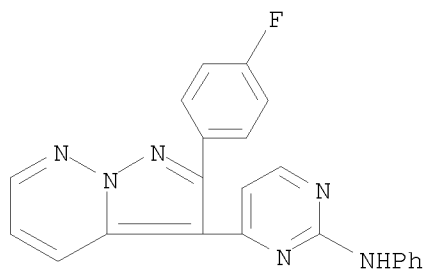
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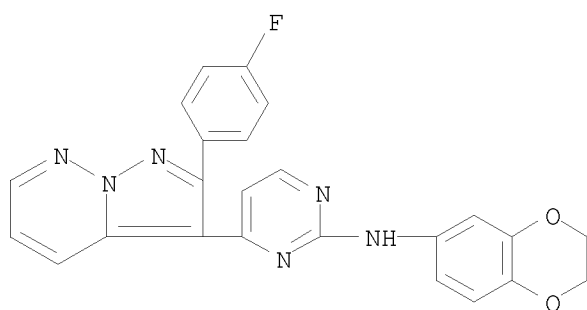


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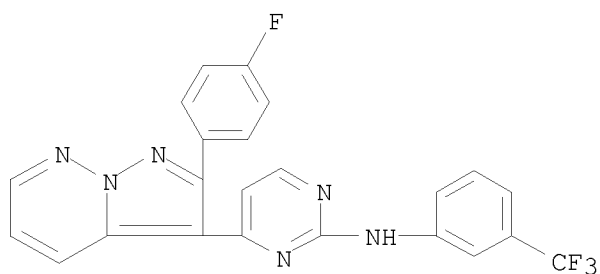
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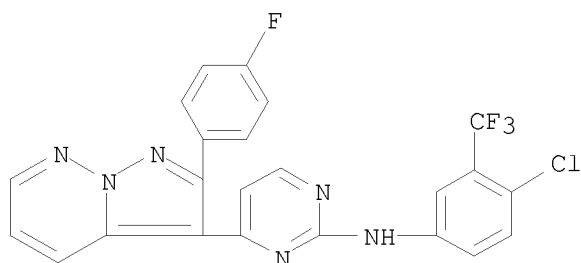
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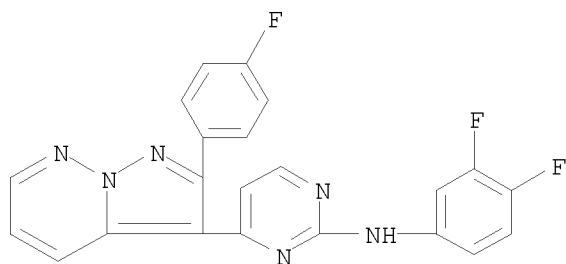
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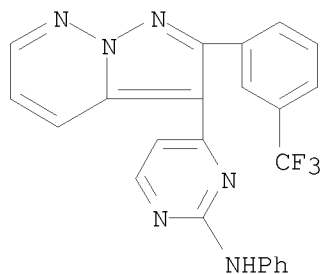
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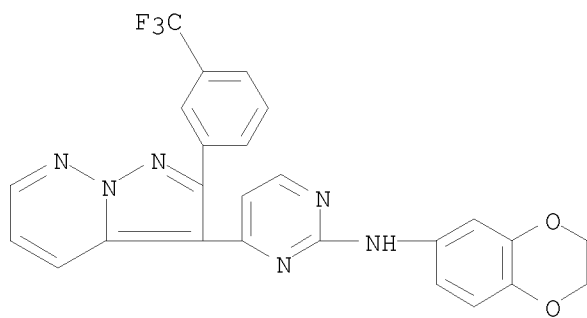
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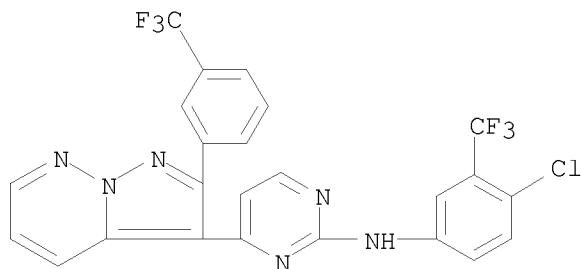
RN 681432-65-5 CAPLUS
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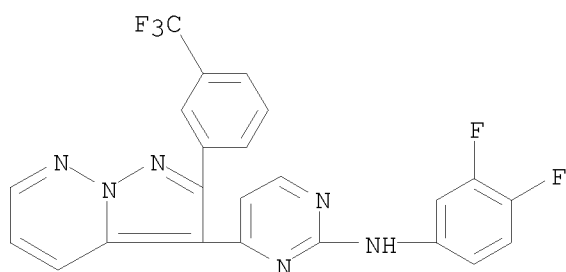
RN 681432-67-7 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



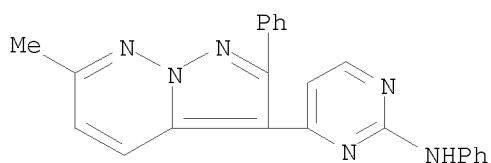
RN 681432-69-9 CAPLUS
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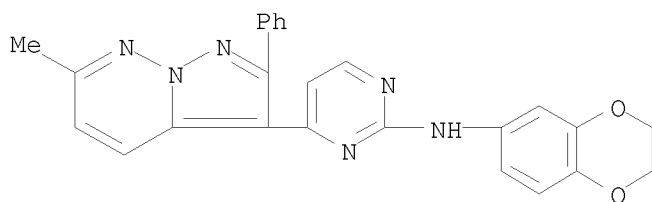
RN 681432-70-2 CAPLUS
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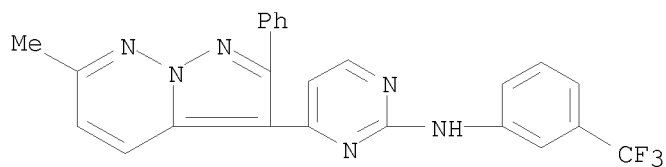
RN 681432-71-3 CAPLUS
 CN 2-Pyrimidinamine, 4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-phenyl- (CA INDEX NAME)



RN 681432-74-6 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)

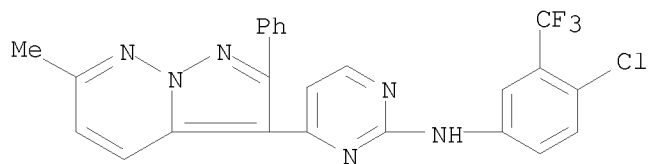


RN 681432-75-7 CAPLUS
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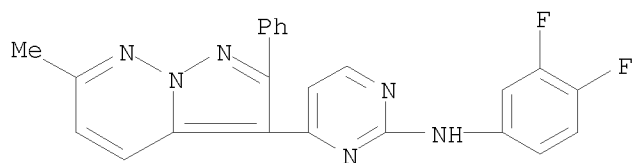
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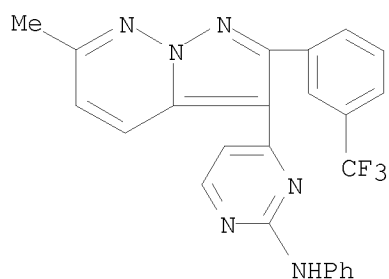
RN 681432-77-9 CAPLUS

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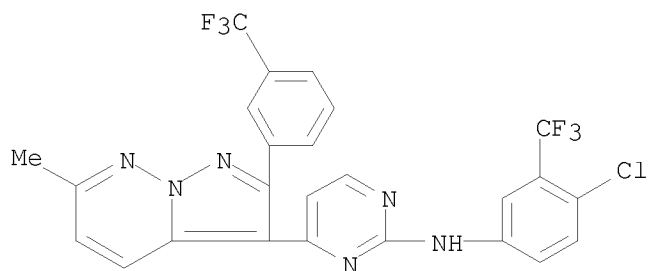
RN 681432-78-0 CAPLUS

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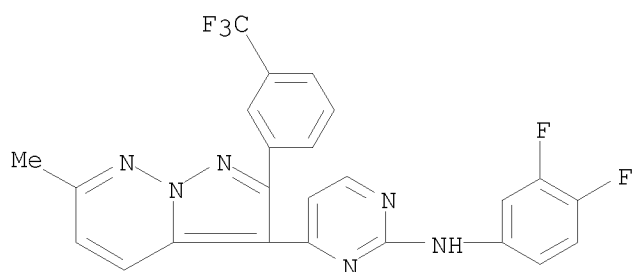


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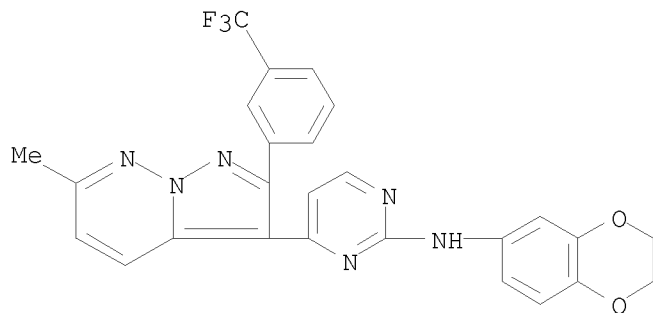
CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



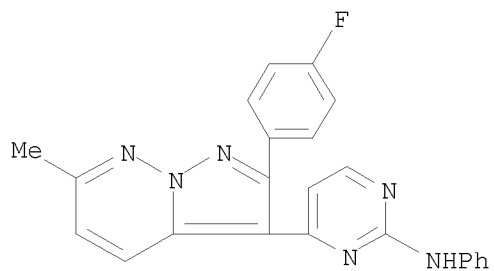
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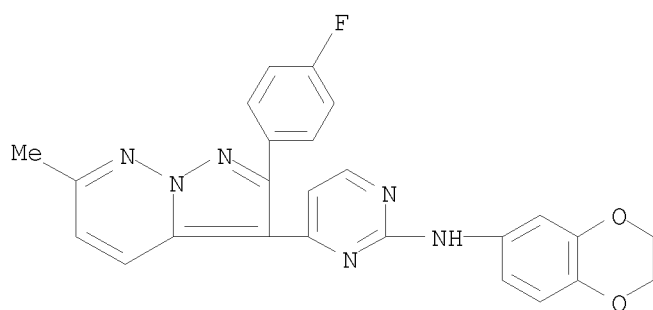
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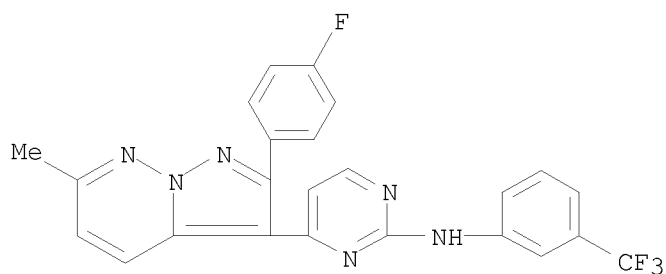
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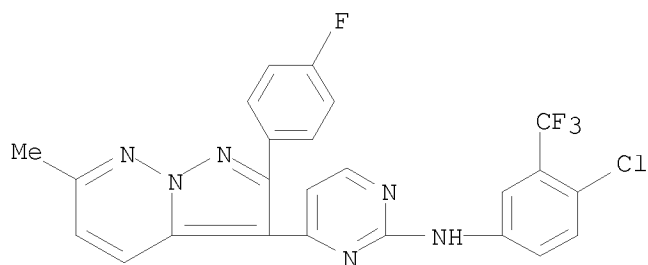
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 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



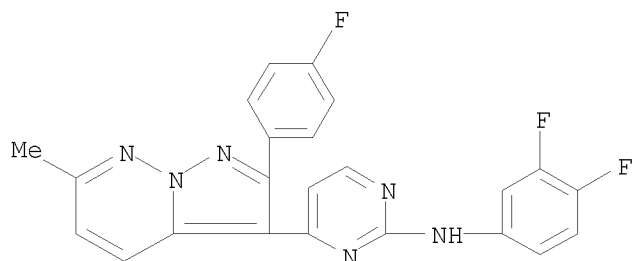
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RN 681432-90-6 CAPLUS
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RN 681432-91-7 CAPLUS
CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ACCESSION NUMBER: 2006:67847 CAPLUS

DOCUMENT NUMBER: 144:285631

TITLE: Inhibitory mode of N-phenyl-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-amine series derivatives against GSK-3: molecular docking and 3D-QSAR analyses

AUTHOR(S): Xiao, Jingfa; Guo, Zongru; Guo, Yanshen; Chu, Fengming; Sun, Piaoyang

CORPORATE SOURCE: Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China

SOURCE: Protein Engineering, Design & Selection (2006), 19(2), 47-54

CODEN: PEDSBR; ISSN: 1741-0126

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Glycogen synthase kinase 3 (GSK-3) inhibition is an important research topic because of its wide range of associated health implications. The interaction mode of a series of N-phenyl-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-amine compds. with human GSK-3 has been studied using mol. docking and 3D-QSAR approaches. In the 3D-QSAR studies, the mol. alignment and conformation determination are so important that they affect the success of a model. Flexible docking (AutoDock3.0.5) was used for the determination of active' conformation and mol. alignment. Comparative mol.

field anal. (CoMFA) and comparative mol. similarity indexes anal. (CoMSIA) were used to develop 3D-QSAR models of 80 N-phenyl-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-amine compds. The r² values were 0.870 and 0.861 for CoMFA and CoMSIA models, resp. The predictive ability of these models was validated by 10 compds. of the test set. Mapping these models back to the topol. of the active site of GSK-3 led to a better understanding of the vital N-phenyl-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-amines-GSK-3 interactions. The results demonstrate that combination of ligand-based and receptor-based modeling is a powerful approach to build 3D-QSAR models. The interaction mode from this study may be helpful for the design of a novel inhibitor and guide the selection of candidate sites for further exptl. studies on site-directed mutagenesis.

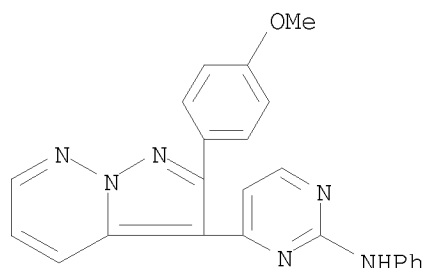
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RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (inhibitory mode of N-Ph-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-amine series derivs. against GSK-3 and mol. docking and 3D-QSAR analyses)

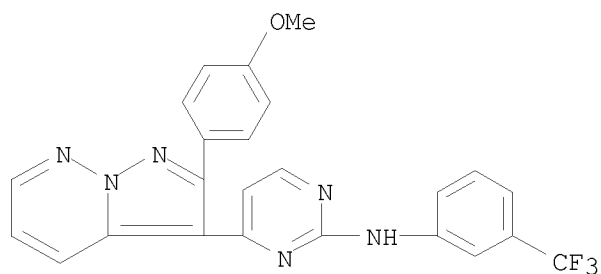
RN 681432-02-0 CAPLUS

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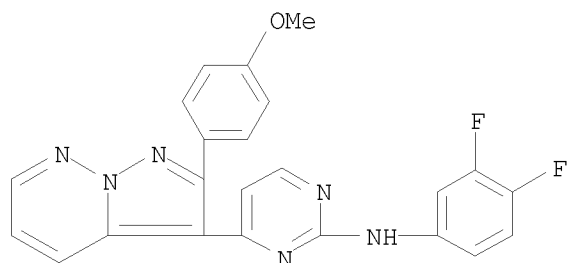
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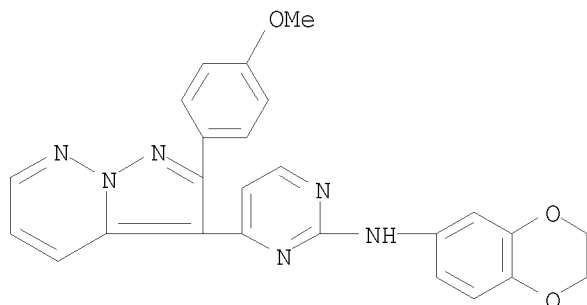


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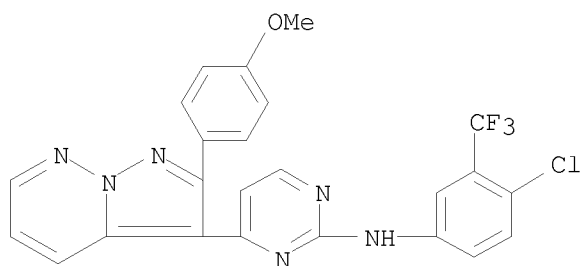
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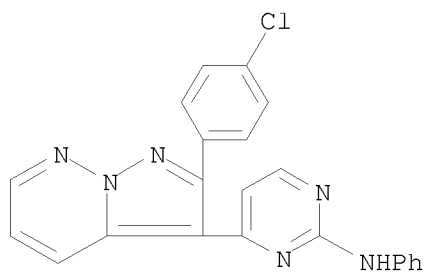
RN 681432-07-5 CAPLUS
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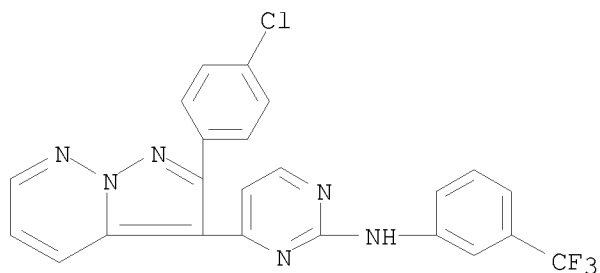
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RN 681432-20-2 CAPLUS
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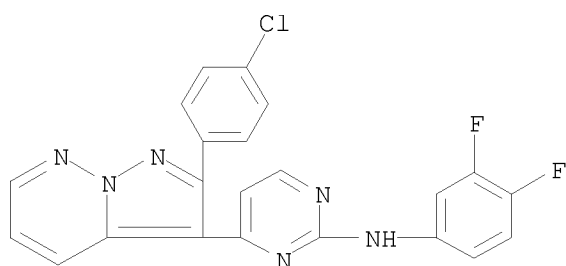


RN 681432-23-5 CAPLUS
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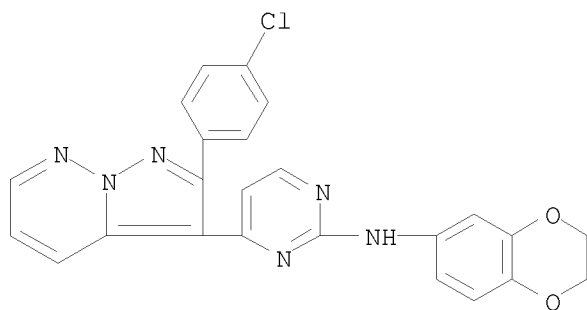
RN 681432-24-6 CAPLUS

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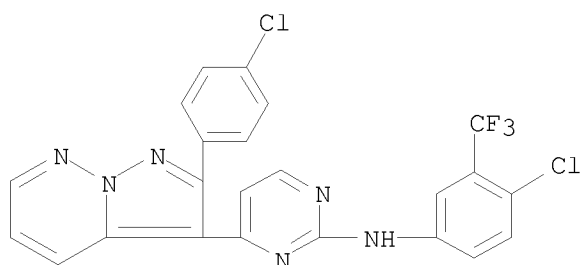
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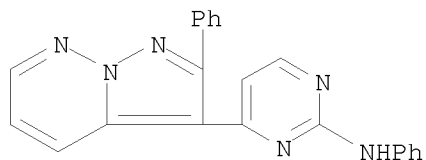


RN 681432-26-8 CAPLUS

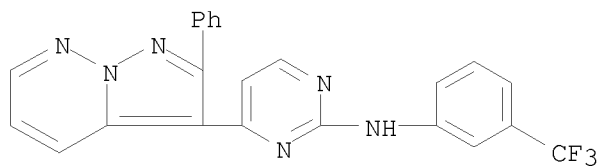
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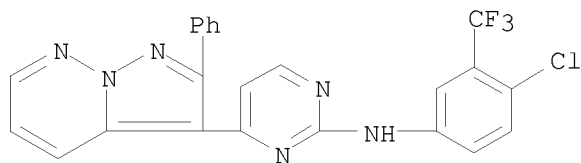
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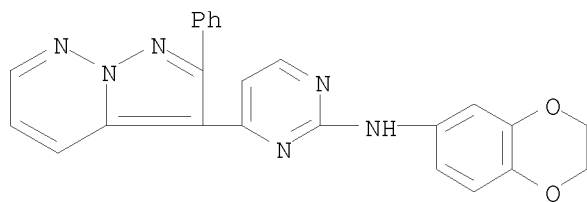
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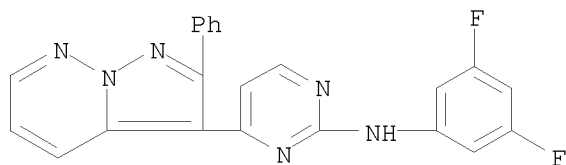
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 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



RN 681432-54-2 CAPLUS
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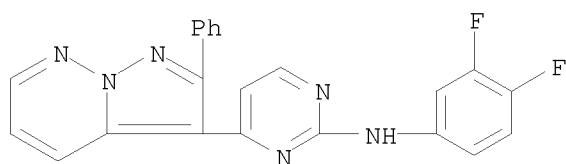


RN 681432-55-3 CAPLUS
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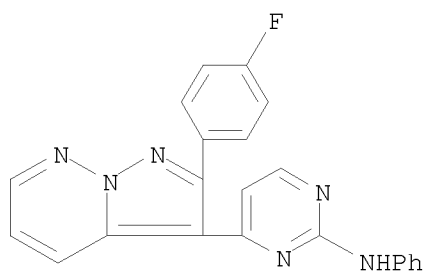
RN 681432-56-4 CAPLUS

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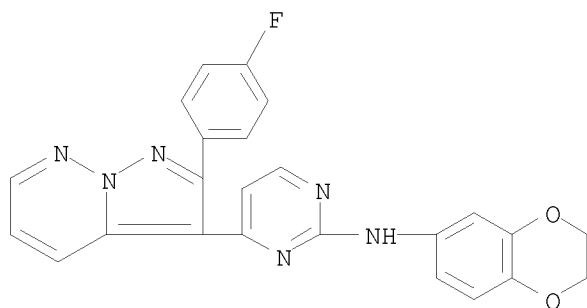
RN 681432-57-5 CAPLUS

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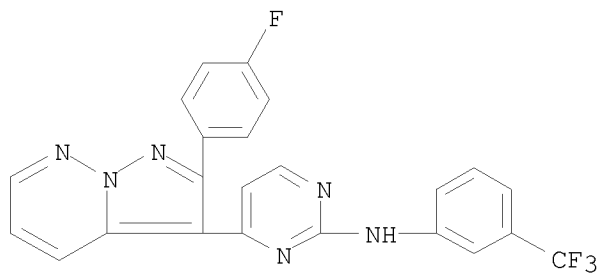
RN 681432-60-0 CAPLUS

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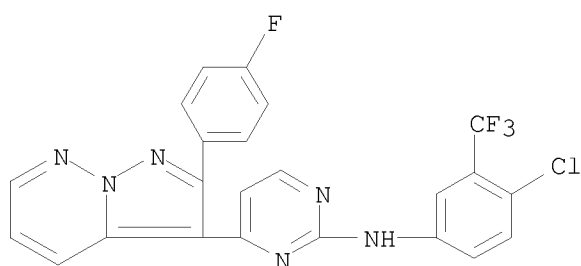
RN 681432-61-1 CAPLUS

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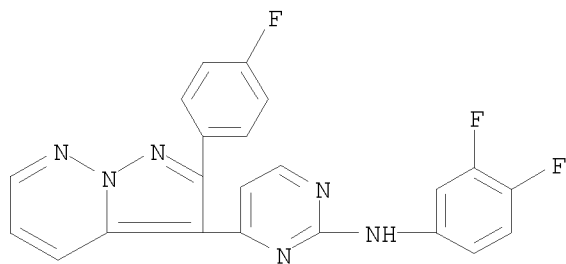
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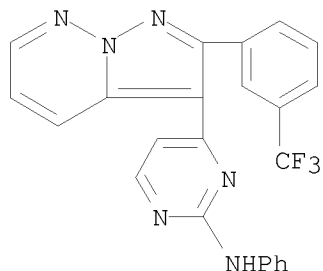
RN 681432-63-3 CAPLUS

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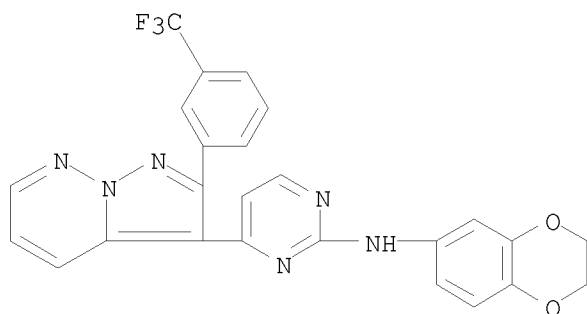


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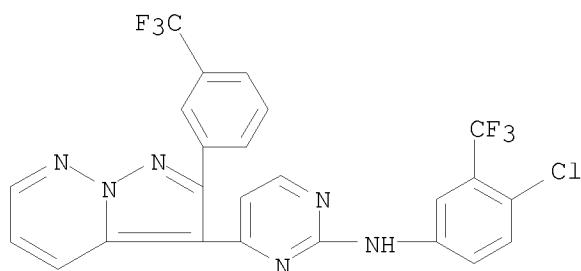
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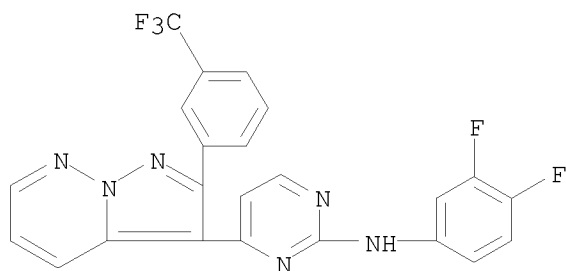
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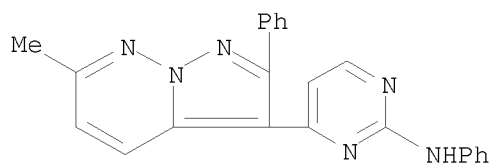
RN 681432-69-9 CAPLUS
 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



RN 681432-70-2 CAPLUS
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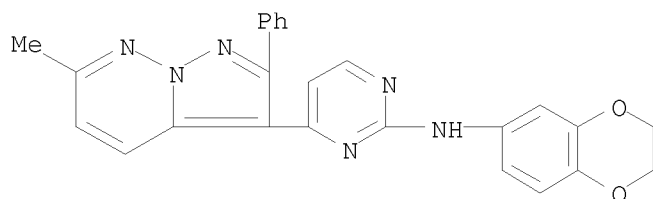


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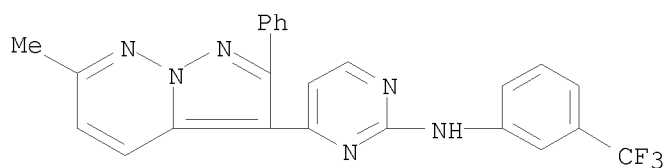
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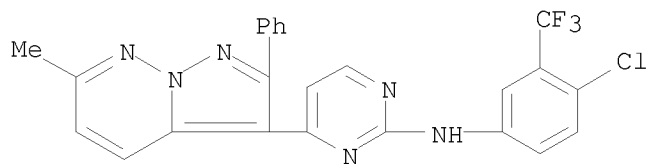
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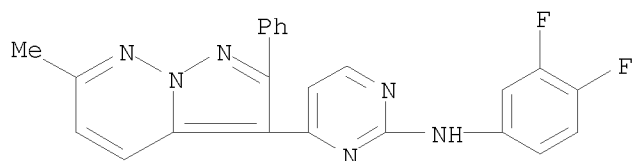
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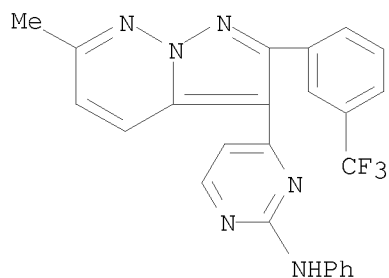


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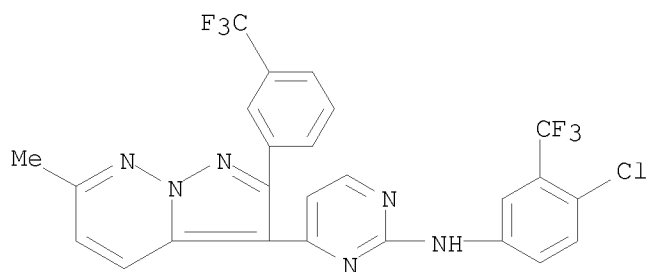
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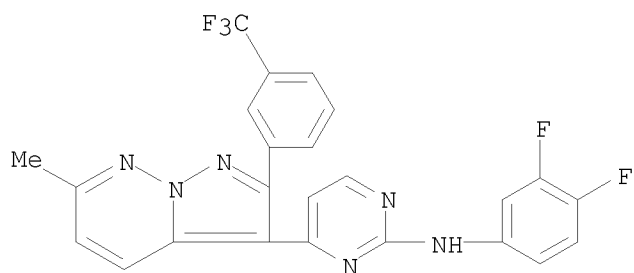
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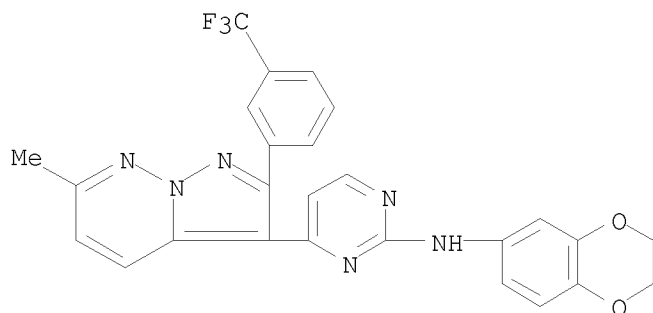
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 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



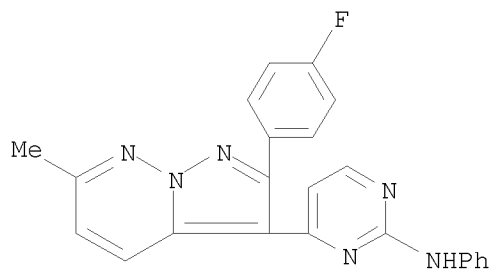
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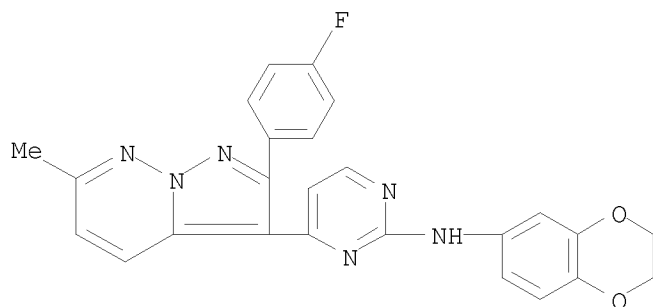
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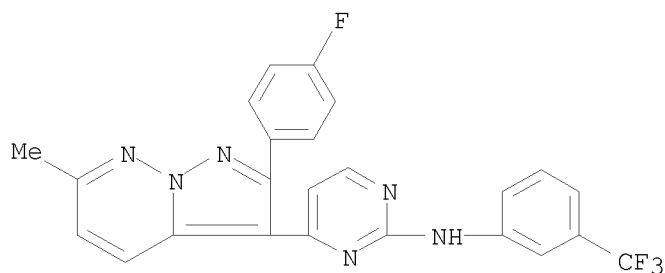
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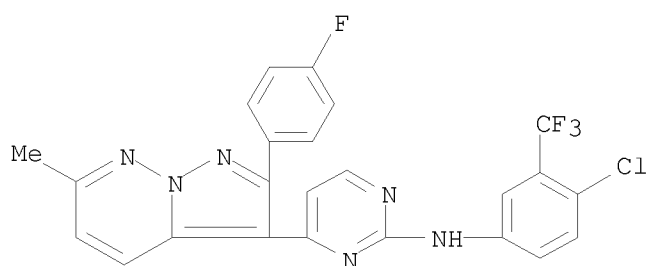
RN 681432-88-2 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



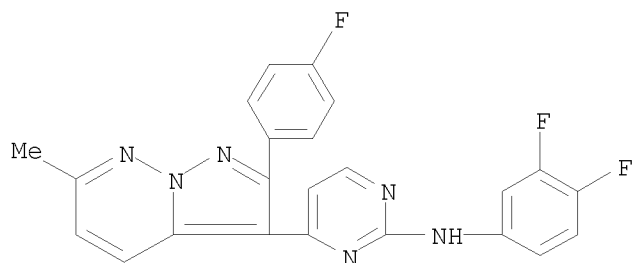
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 CN 2-Pyrimidinamine, 4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 681432-90-6 CAPLUS
 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



RN 681432-91-7 CAPLUS
 CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:650360 CAPLUS
 DOCUMENT NUMBER: 141:218318
 TITLE: N-Phenyl-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-
 amines as Potent and Selective Inhibitors of Glycogen
 Synthase Kinase 3 with Good Cellular Efficacy
 AUTHOR(S): Tavares, Francis X.; Boucheron, Joyce A.; Dickerson,
 Scott H.; Griffin, Robert J.; Preugschat, Frank;
 Thomson, Stephen A.; Wang, Tony Y.; Zhou, Hui-Qiang
 CORPORATE SOURCE: Department of Medicinal Chemistry, GlaxoSmithKline,
 Research Triangle Park, NC, 27709, USA
 SOURCE: Journal of Medicinal Chemistry (2004), 47(19),
 4716-4730
 CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:218318

AB Glycogen synthase kinase 3 regulates glycogen synthase, the rate-determining enzyme for glycogen synthesis. Liver and muscle glycogen synthesis is defective in type 2 diabetics, resulting in elevated plasma glucose levels. Inhibition of GSK-3 could potentially be an effective method to control plasma glucose levels in type 2 diabetics. Structure-activity studies on a N-phenyl-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-amine series have led to the identification of potent and selective compds. with good cellular efficacy. Mol. modeling studies have given insights into the mode of binding of these inhibitors. Since the initial leads were also potent inhibitors of CDK-2/CDK-4, an extensive SAR was performed at various positions of the pyrazolo[1,5-b]pyridazin core to afford potent GSK-3 inhibitors that were highly selective over CDK-2. In addition, these inhibitors also exhibited very good cell efficacy and functional response. A representative example was shown to have good oral exposure levels, extending their utility in an in vivo setting. These inhibitors provide a viable lead series in the discovery of new therapies for the treatment of type 2 diabetes.

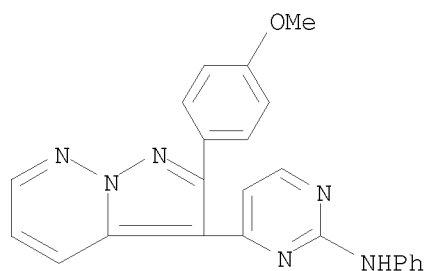
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RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

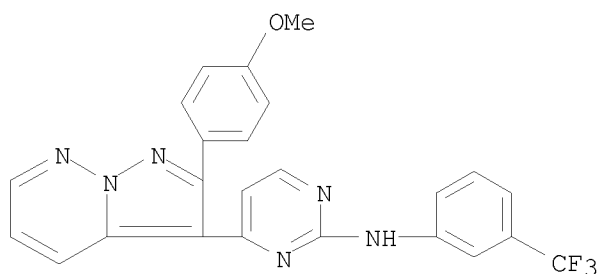
(N-Ph-4-pyrazolo[1,5-b]pyridazin-3-ylpyrimidin-2-amines as potent and selective inhibitors of glycogen synthase kinase 3 with good cellular efficacy)

RN 681432-02-0 CAPLUS

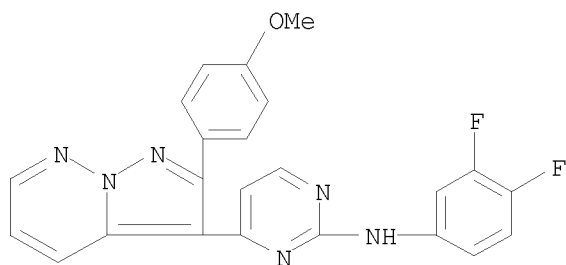
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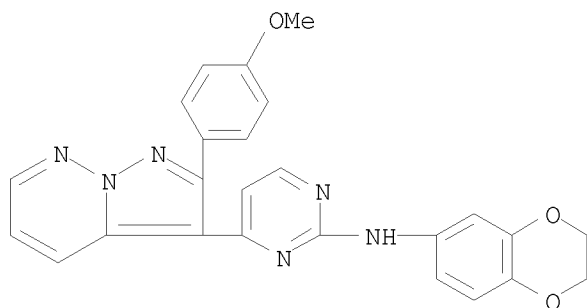
RN 681432-05-3 CAPLUS
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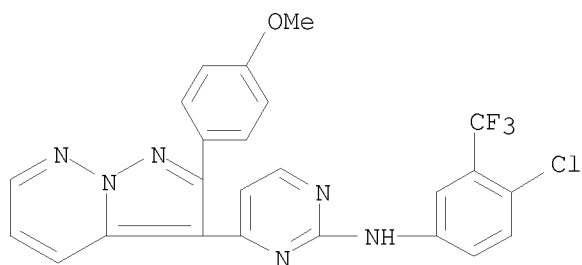
RN 681432-06-4 CAPLUS
CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



RN 681432-07-5 CAPLUS
CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)

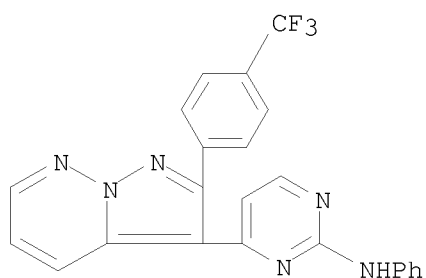


RN 681432-10-0 CAPLUS
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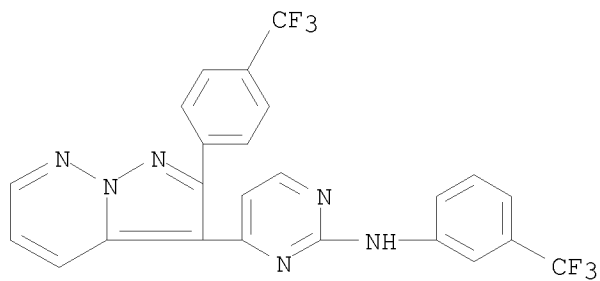
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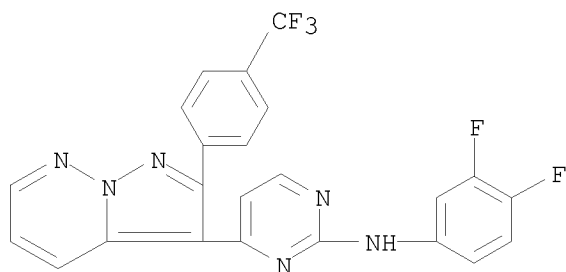
RN 681432-16-6 CAPLUS

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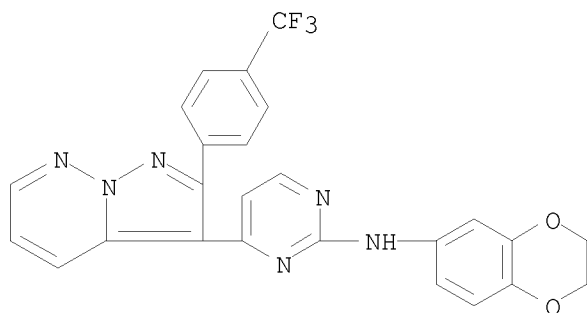


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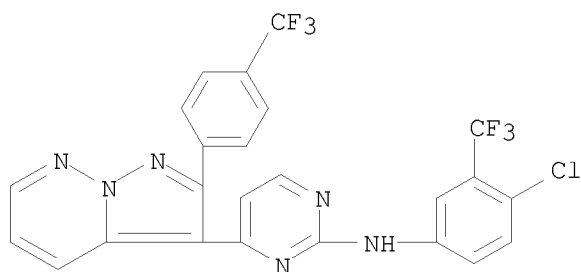
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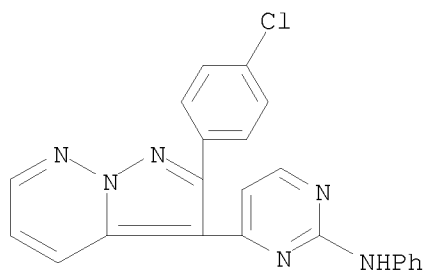
RN 681432-18-8 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



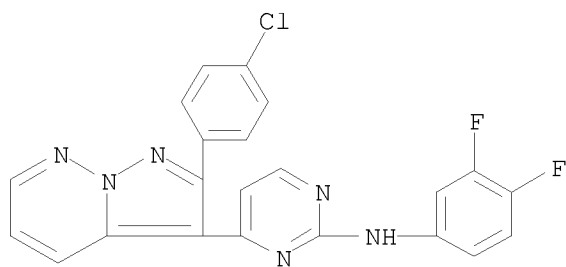
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RN 681432-20-2 CAPLUS
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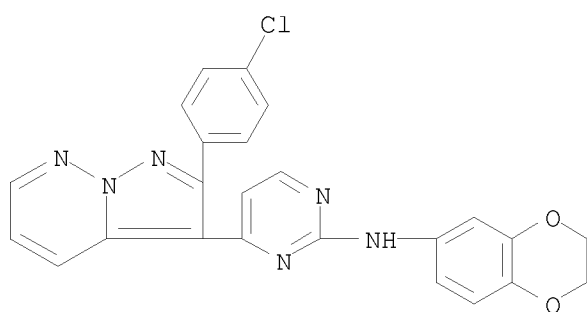


RN 681432-24-6 CAPLUS
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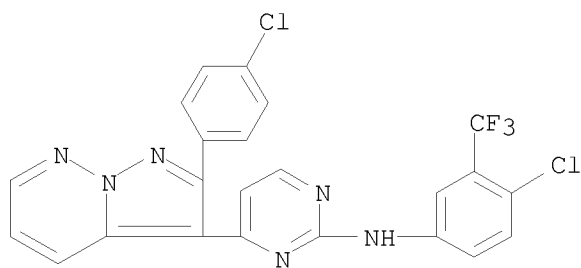
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CN 2-Pyrimidinamine, 4-[2-(4-chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-(2,3-dihydro-1,4-benzodioxin-6-yl)- (CA INDEX NAME)



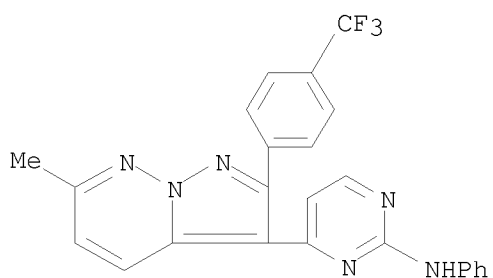
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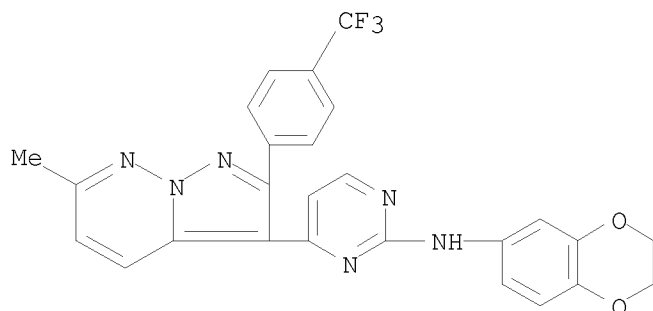


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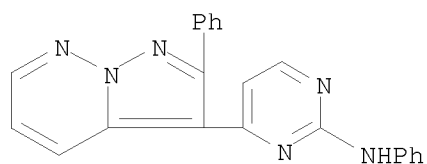
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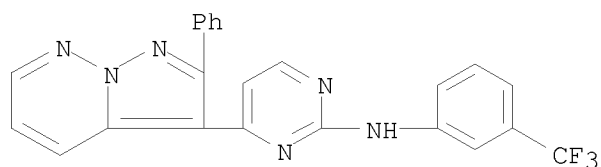
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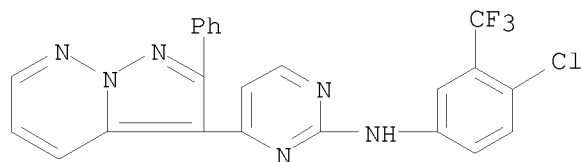
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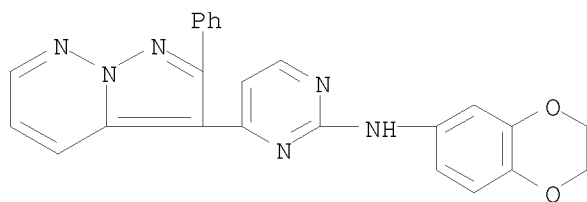
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RN 681432-53-1 CAPLUS
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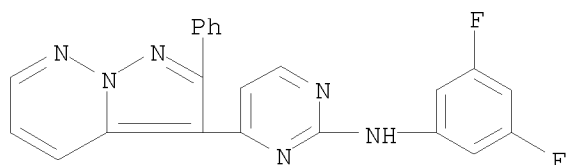


RN 681432-54-2 CAPLUS
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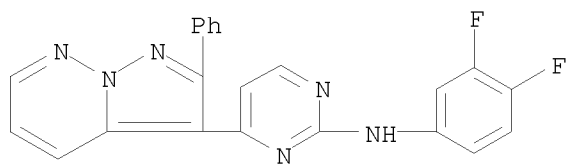
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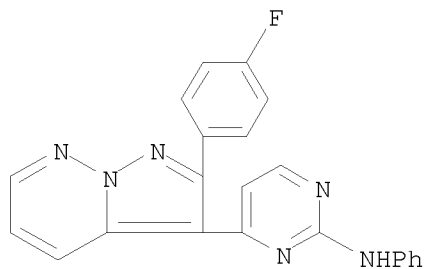
RN 681432-56-4 CAPLUS

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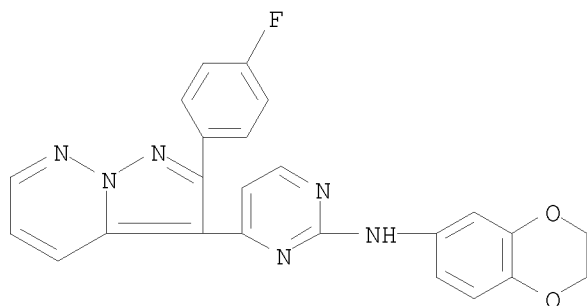
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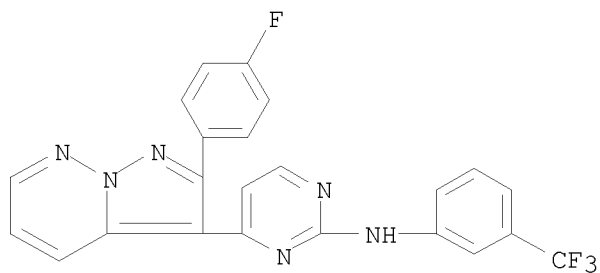
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CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



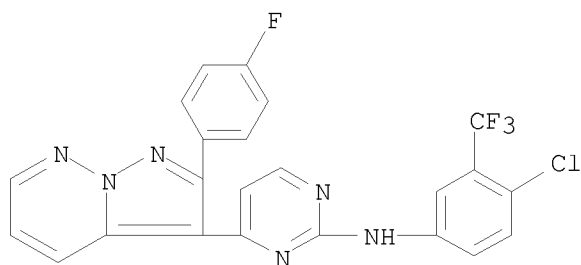
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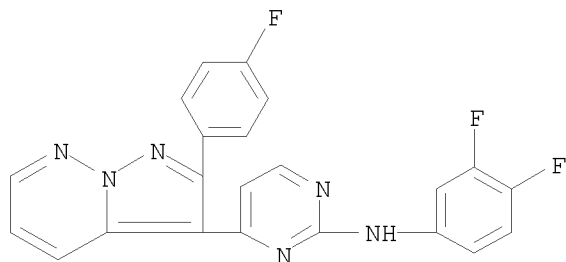
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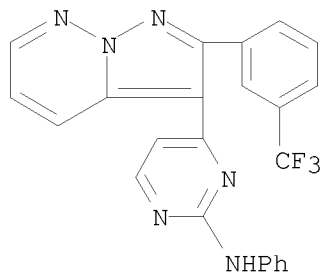


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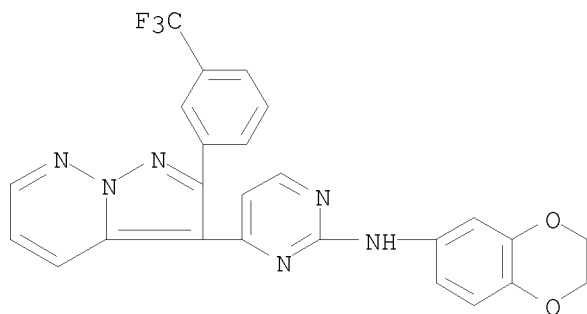
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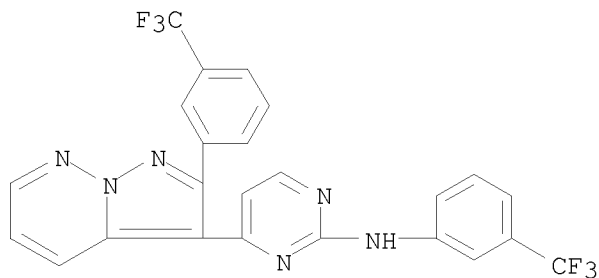
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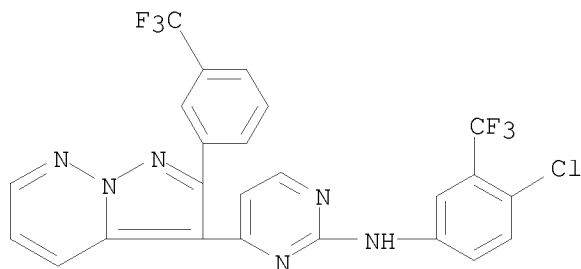
RN 681432-67-7 CAPLUS
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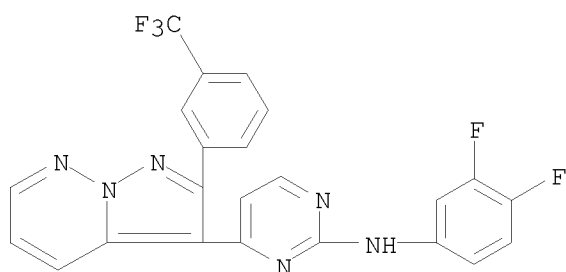
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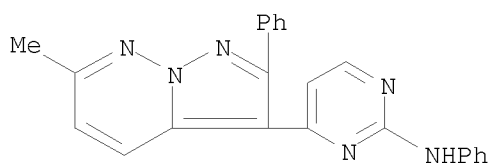
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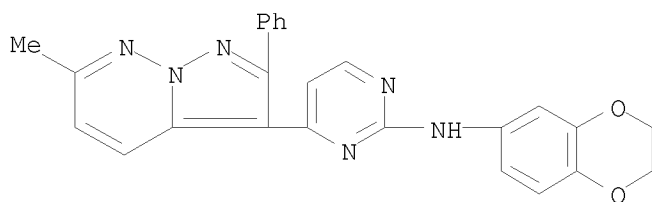
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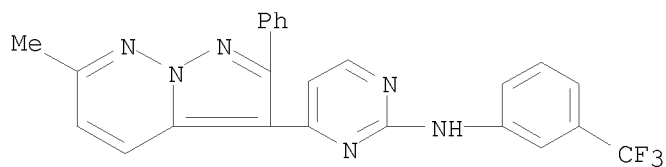
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RN 681432-74-6 CAPLUS
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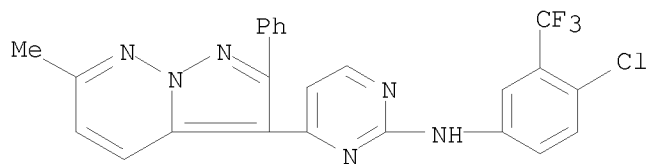


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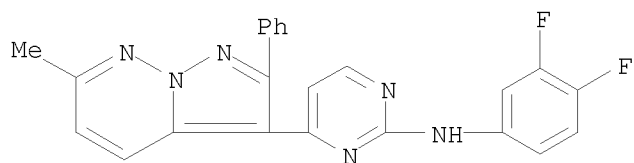
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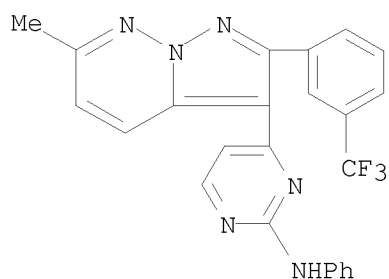
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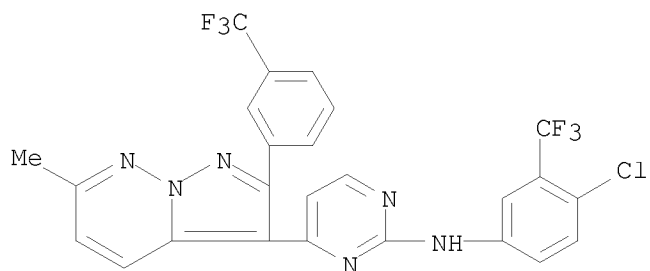
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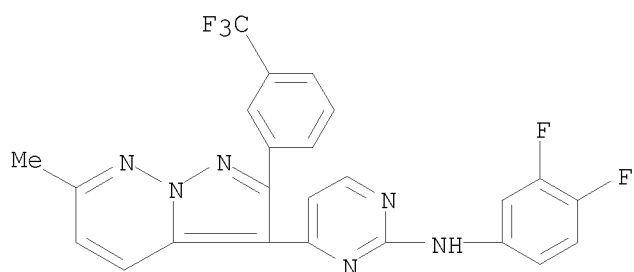


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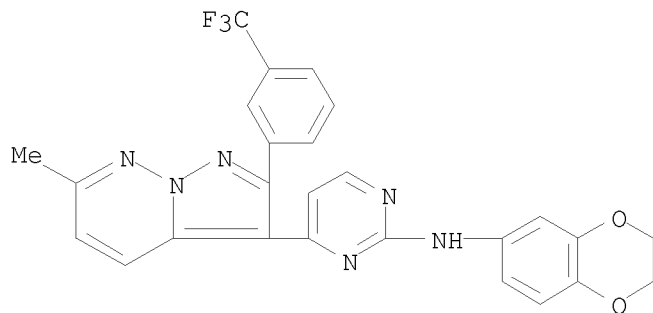
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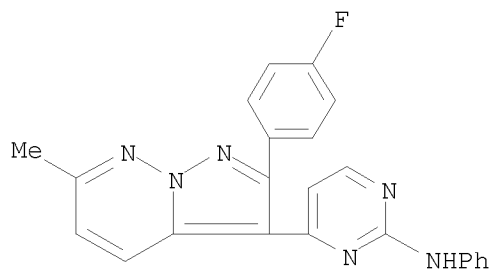
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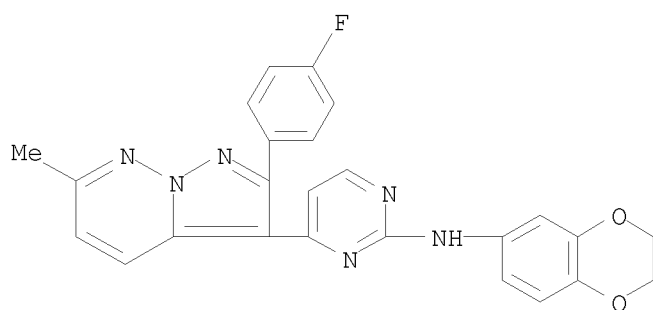
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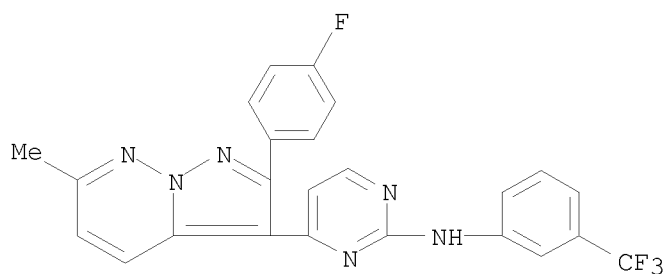
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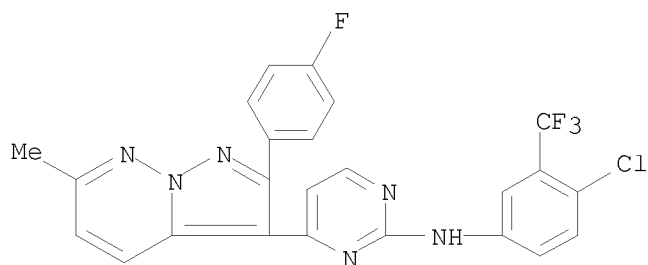
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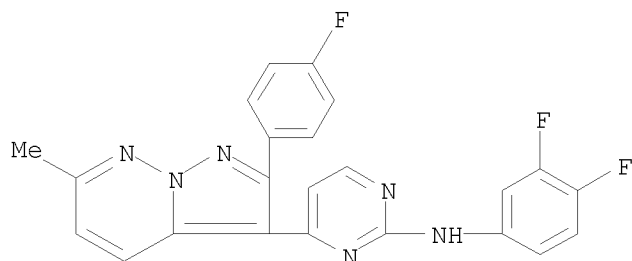
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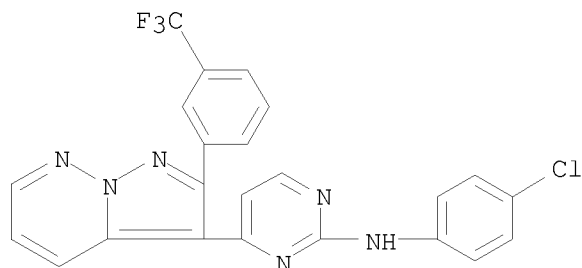
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RN 681432-91-7 CAPLUS
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RN 748142-00-9 CAPLUS
 CN 2-Pyrimidinamine, N-(4-chlorophenyl)-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:354948 CAPLUS
 DOCUMENT NUMBER: 140:357361
 TITLE: Preparation of pyrazolopyridazines as GSK-3 kinase inhibitors for treating Type II Diabetes
 INVENTOR(S): Dickerson, Scott Howard; Tavares, Francis Xavier; Zhou, Huiqiang
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
 SOURCE: PCT Int. Appl., 136 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035588	A1	20040429	WO 2003-US32473	20031014
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KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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 US 2006069097 A1 20060330 US 2005-530985 20050412
 PRIORITY APPLN. INFO.: US 2002-418522P P 20021015
 WO 2003-US32473 W 20031014
 OTHER SOURCE(S): MARPAT 140:357361
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein D = N, CH; R1 = (un)substituted hetero/aryl; n =
 1 or 2; R2 = H, alk(en/yn)yl, haloalkyl, cycloalkyl, halo, heterocyclyl,
 hetero/aryl, CN, azido, NO2, OH and derivs., CO2H and derivs., CONH2 and
 derivs., NH2 and derivs. S(O)qH and derivs., etc.; q = 0-2; R3 = Qp-Q1; Q
 = O, NH and derivs., S(O)q; p = 0 or 1; Q1 = ar/cyclo/halo/alkyl,
 heteroaryl, (un)substituted aryl, etc.; their salts, solvates, and
 physiol. functional derivs.] were prepared as GSK3 kinase inhibitors for
 treating Type II Diabetes mellitus. For example, II was prepared by
 cycloaddn. of 1-aminopyridazin-3-yl iodide (preparation given) with 3-butyn-2-one
 in CH2Cl2, reaction of the methylketone with DMF di-tert-butylacetal in
 DMF, and cyclocondensation of the α , β -unsatd. ketone with
 N-cyclopropylguanidine•0.5H2SO4 (preparation given) in DMF in the presence
 of K2CO3. I displayed pIC50 values > 5.0 for the inhibition of GSK3
 kinase.
 IT 681432-02-0P, 4-[2-(4-Methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]-
 N-phenylpyrimidin-2-amine 681432-05-3P, 4-[2-(4-
 Methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-[3-
 (trifluoromethyl)phenyl]pyrimidin-2-amine 681432-06-4P,
 N-(3,4-Difluorophenyl)-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-
 yl]pyrimidin-2-amine 681432-07-5P, N-(2,3-Dihydro-1,4-
 benzodioxin-6-yl)-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-
 yl]pyrimidin-2-amine 681432-10-0P, N-[4-Chloro-3-
 (trifluoromethyl)phenyl]-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-
 yl]pyrimidin-2-amine 681432-12-2P, N-Phenyl-4-[2-[4-
 (trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]pyrimidin-2-amine
 681432-16-6P, N-[3-(Trifluoromethyl)phenyl]-4-[2-[4-
 (trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]pyrimidin-2-amine
 681432-17-7P, N-(3,4-Difluorophenyl)-4-[2-[4-
 (trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]pyrimidin-2-amine
 681432-18-8P, N-(2,3-Dihydro-1,4-benzodioxin-6-yl)-4-[2-[4-
 (trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]pyrimidin-2-amine
 681432-19-9P, N-[4-Chloro-3-(trifluoromethyl)phenyl]-4-[2-[4-
 (trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]pyrimidin-2-amine
 681432-20-2P, 4-[2-(4-Chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-
 N-phenylpyrimidin-2-amine 681432-23-5P, 4-[2-(4-
 Chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-[3-
 (trifluoromethyl)phenyl]pyrimidin-2-amine 681432-24-6P,
 4-[2-(4-Chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-(3,4-
 difluorophenyl)pyrimidin-2-amine 681432-25-7P,
 4-[2-(4-Chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-(2,3-dihydro-1,4-
 benzodioxin-6-yl)pyrimidin-2-amine 681432-26-8P,
 4-[2-(4-Chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-[4-chloro-3-
 (trifluoromethyl)phenyl]pyrimidin-2-amine 681432-27-9P,

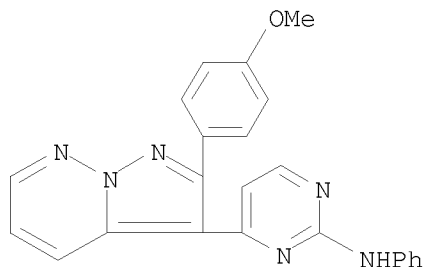
4-[6-Methyl-2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-N-phenylpyrimidin-2-amine 681432-30-4P 681432-49-5P,
N-Phenyl-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-2-pyrimidinamine 681432-52-0P, 4-(2-Phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-[3-(trifluoromethyl)phenyl]-2-pyrimidinamine 681432-53-1P,
N-[4-Chloro-3-(trifluoromethyl)phenyl]-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-2-pyrimidinamine 681432-54-2P, N-(2,3-Dihydro-1,4-benzodioxin-6-yl)-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-2-pyrimidinamine 681432-55-3P, N-(3,5-Difluorophenyl)-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-2-pyrimidinamine 681432-56-4P
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N-(2,3-Dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-61-1P,
4-[2-(4-Fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]-2-pyrimidinamine 681432-62-2P,
N-[4-Chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-63-3P,
N-(3,4-Difluorophenyl)-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-65-5P, N-Phenyl-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-67-7P, N-(2,3-Dihydro-1,4-benzodioxin-6-yl)-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-68-8P, N-[3-(Trifluoromethyl)phenyl]-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-69-9P, N-[4-Chloro-3-(trifluoromethyl)phenyl]-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-70-2P, N-(3,4-Difluorophenyl)-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-71-3P, 4-(6-Methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-phenyl-2-pyrimidinamine 681432-74-6P, N-(2,3-Dihydro-1,4-benzodioxin-6-yl)-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-2-pyrimidinamine 681432-75-7P, 4-(6-Methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-[3-(trifluoromethyl)phenyl]-2-pyrimidinamine 681432-76-8P, N-[4-Chloro-3-(trifluoromethyl)phenyl]-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-2-pyrimidinamine 681432-77-9P
, N-(3,4-Difluorophenyl)-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-2-pyrimidinamine 681432-78-0P, 4-[6-Methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl-2-pyrimidinamine 681432-81-5P, 4-[6-Methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]-2-pyrimidinamine 681432-82-6P,
N-[4-Chloro-3-(trifluoromethyl)phenyl]-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-83-7P, N-(3,4-Difluorophenyl)-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-84-8P, N-(2,3-Dihydro-1,4-benzodioxin-6-yl)-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-85-9P, 4-[2-(4-Fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl-2-pyrimidinamine 681432-88-2P,
N-(2,3-Dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-89-3P
, 4-[2-(4-Fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]-2-pyrimidinamine 681432-90-6P,
N-[4-Chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine 681432-91-7P
, N-(3,4-Difluorophenyl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-2-pyrimidinamine

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(GSK3 inhibitor; preparation of pyrazolopyridazines as GSK-3 inhibitors for treating Type II Diabetes)

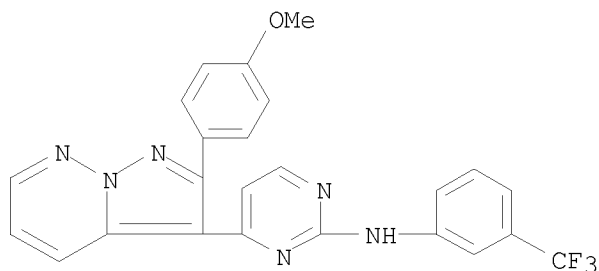
RN 681432-02-0 CAPLUS

CN 2-Pyrimidinamine, 4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl- (CA INDEX NAME)



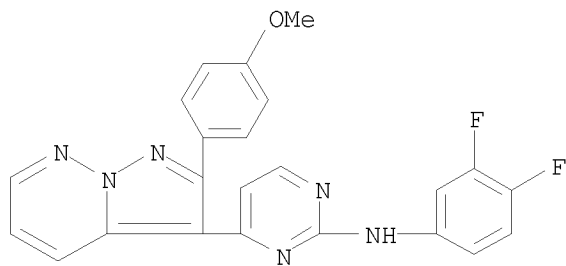
RN 681432-05-3 CAPLUS

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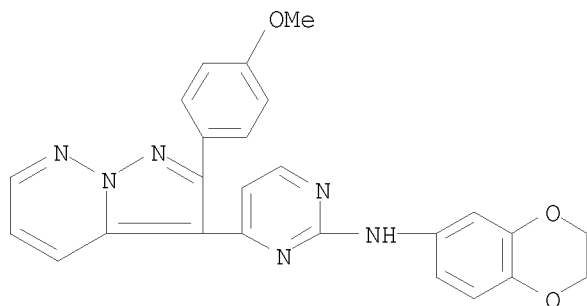
RN 681432-06-4 CAPLUS

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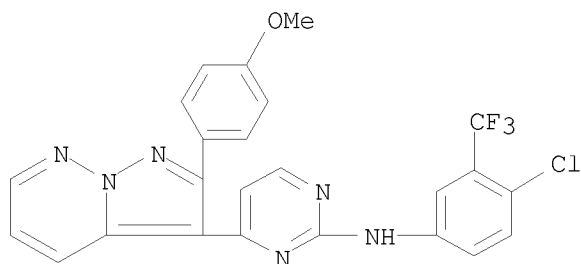
RN 681432-07-5 CAPLUS

CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



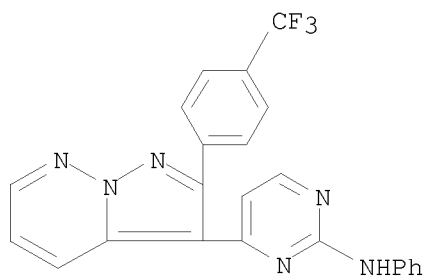
RN 681432-10-0 CAPLUS

CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-methoxyphenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



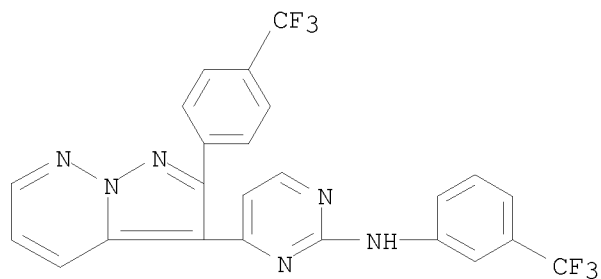
RN 681432-12-2 CAPLUS

CN 2-Pyrimidinamine, N-phenyl-4-[2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)

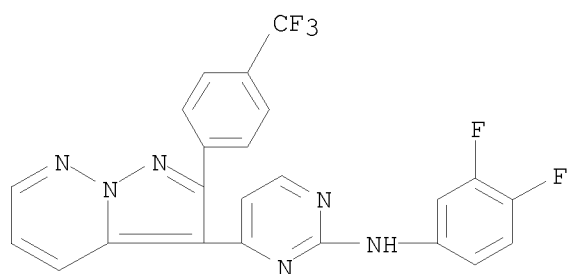


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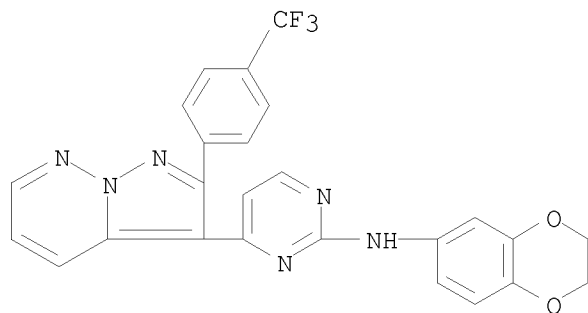
CN 2-Pyrimidinamine, N-[3-(trifluoromethyl)phenyl]-4-[2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



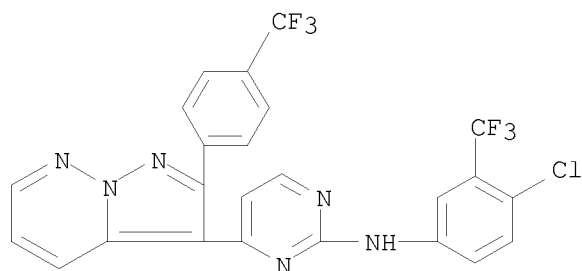
RN 681432-17-7 CAPLUS
 CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-[2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



RN 681432-18-8 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)

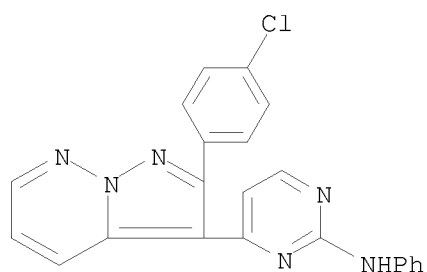


RN 681432-19-9 CAPLUS
 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



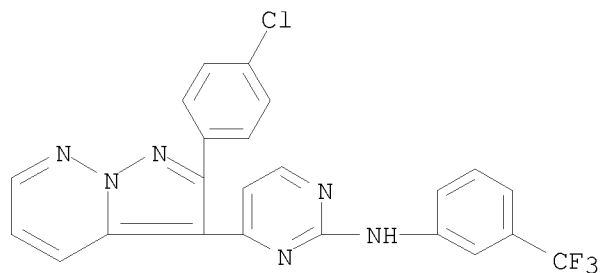
RN 681432-20-2 CAPLUS

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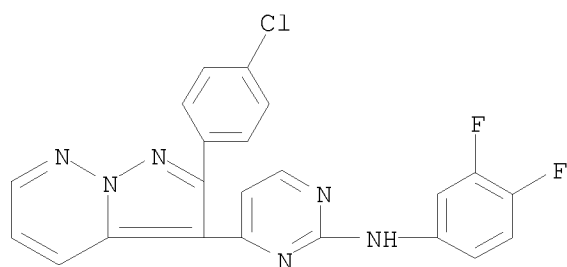
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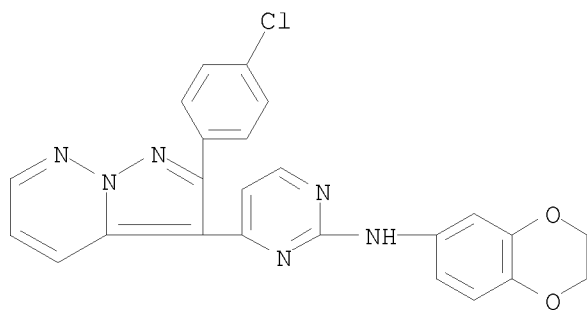


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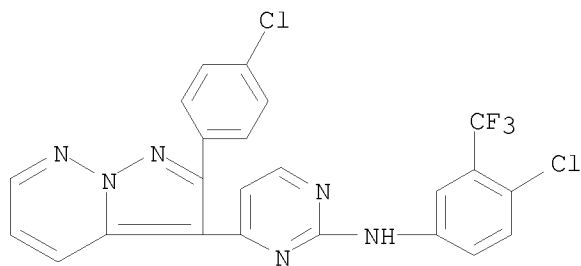
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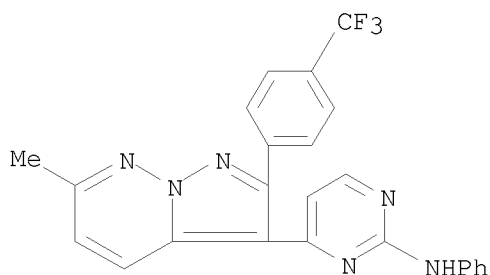
RN 681432-25-7 CAPLUS
 CN 2-Pyrimidinamine, 4-[2-(4-chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-(2,3-dihydro-1,4-benzodioxin-6-yl)- (CA INDEX NAME)



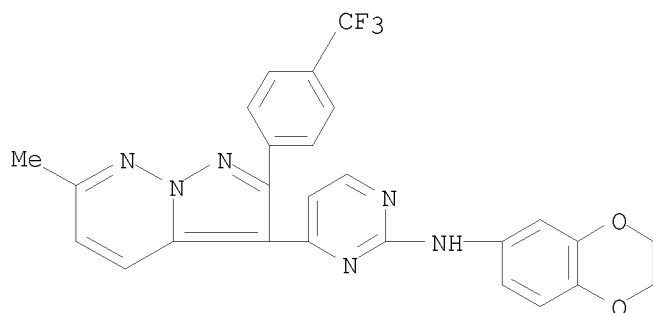
RN 681432-26-8 CAPLUS
 CN 2-Pyrimidinamine, 4-[2-(4-chlorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]-N-[4-chloro-3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



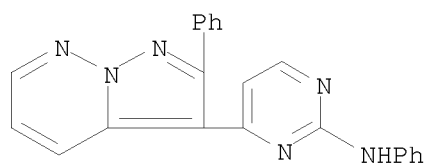
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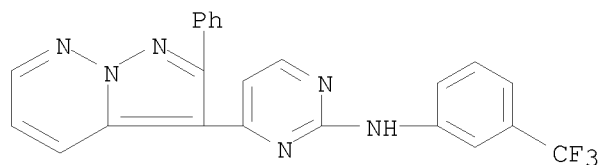
RN 681432-30-4 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[6-methyl-2-[4-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



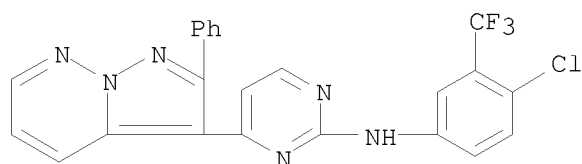
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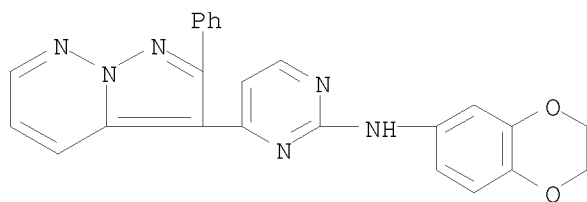
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RN 681432-53-1 CAPLUS
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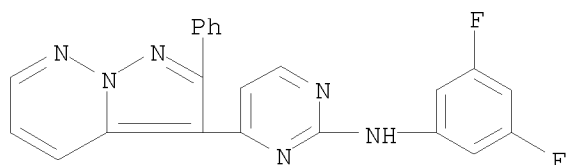


RN 681432-54-2 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



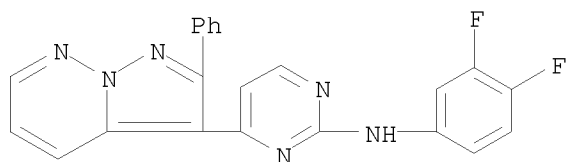
RN 681432-55-3 CAPLUS

CN 2-Pyrimidinamine, N-(3,5-difluorophenyl)-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



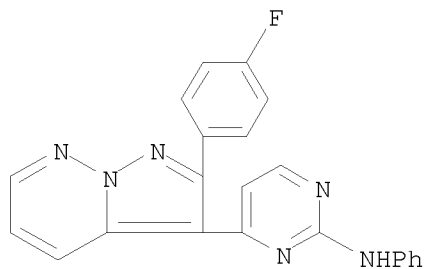
RN 681432-56-4 CAPLUS

CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-(2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



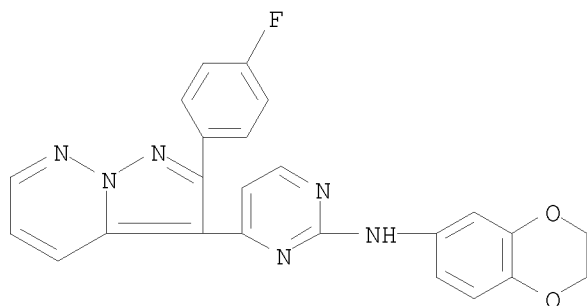
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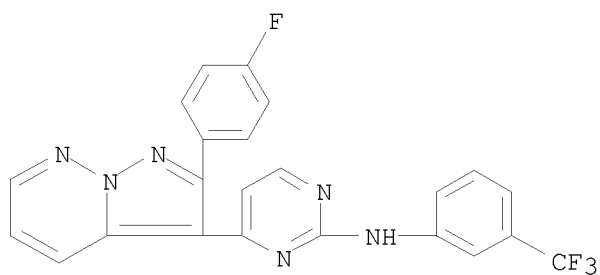
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CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



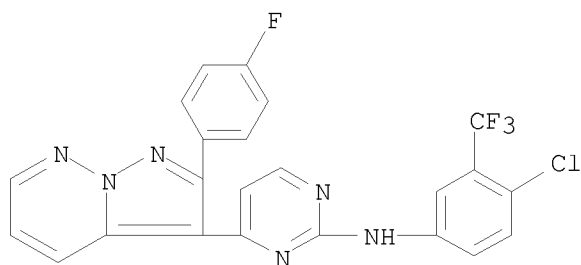
RN 681432-61-1 CAPLUS

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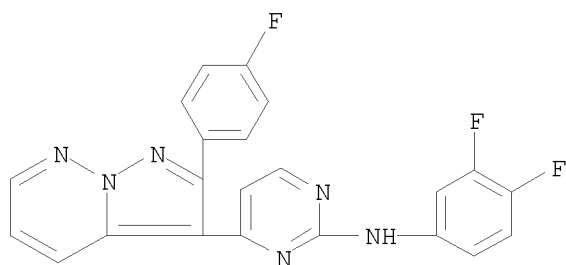
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CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)

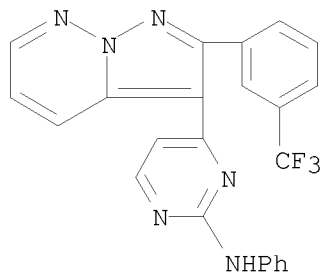


RN 681432-63-3 CAPLUS

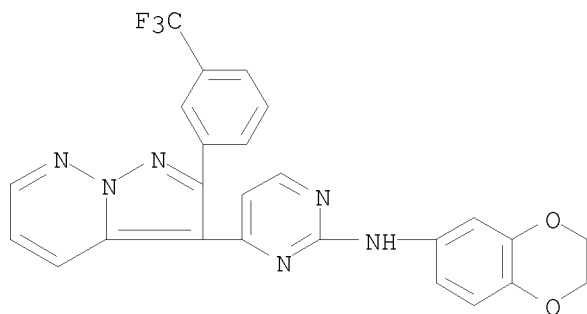
CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-[2-(4-fluorophenyl)pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



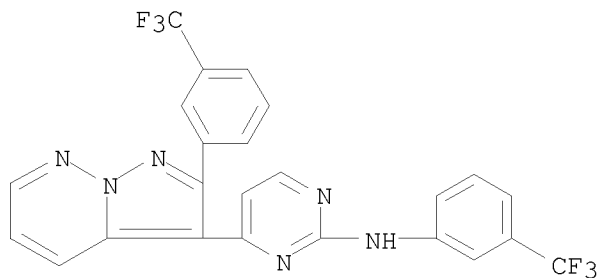
RN 681432-65-5 CAPLUS
 CN 2-Pyrimidinamine, N-phenyl-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



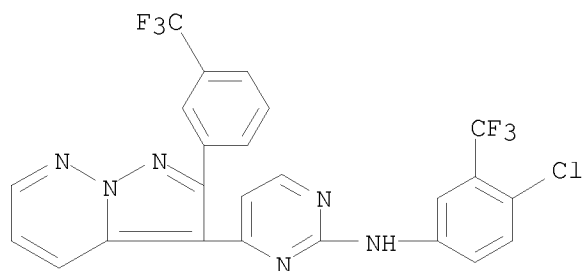
RN 681432-67-7 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



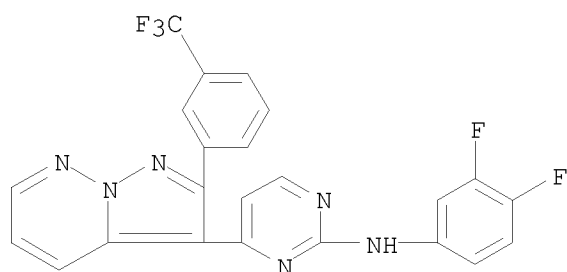
RN 681432-68-8 CAPLUS
 CN 2-Pyrimidinamine, N-[3-(trifluoromethyl)phenyl]-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



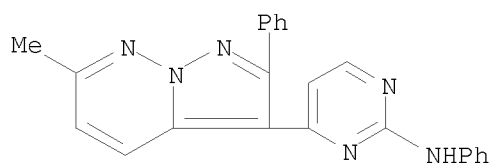
RN 681432-69-9 CAPLUS
 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



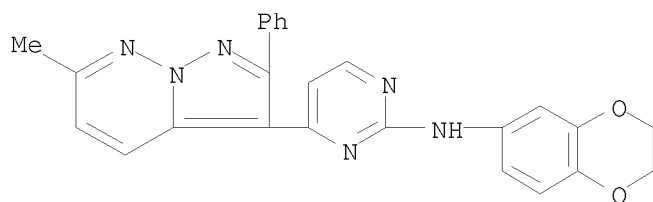
RN 681432-70-2 CAPLUS
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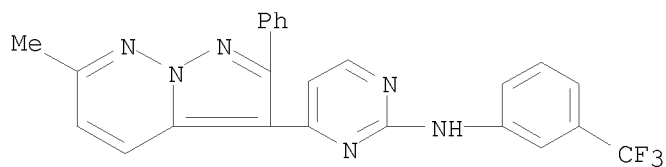
RN 681432-71-3 CAPLUS
 CN 2-Pyrimidinamine, 4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-phenyl- (CA INDEX NAME)



RN 681432-74-6 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)

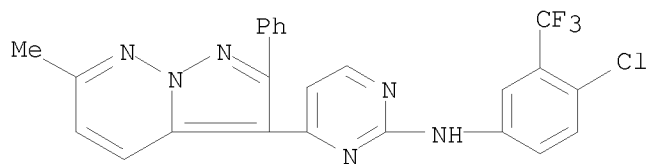


RN 681432-75-7 CAPLUS
 CN 2-Pyrimidinamine, 4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



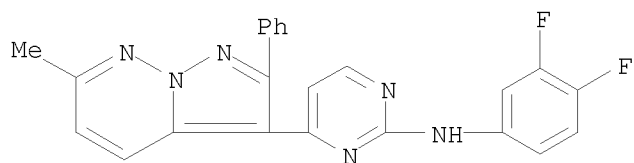
RN 681432-76-8 CAPLUS

CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



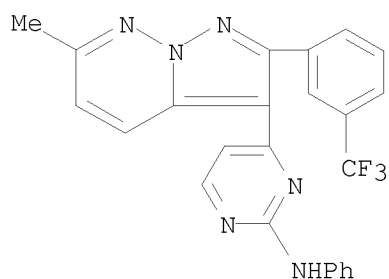
RN 681432-77-9 CAPLUS

CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-(6-methyl-2-phenylpyrazolo[1,5-b]pyridazin-3-yl)- (CA INDEX NAME)



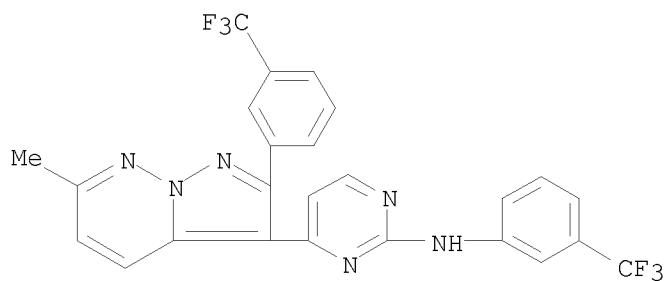
RN 681432-78-0 CAPLUS

CN 2-Pyrimidinamine, 4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl- (CA INDEX NAME)



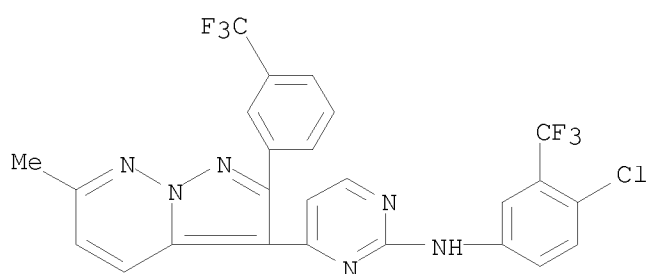
RN 681432-81-5 CAPLUS

CN 2-Pyrimidinamine, 4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



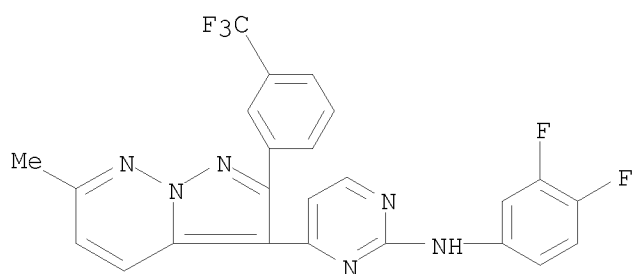
RN 681432-82-6 CAPLUS

CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



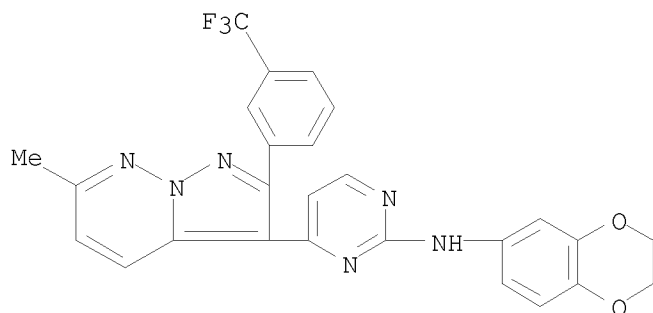
RN 681432-83-7 CAPLUS

CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)

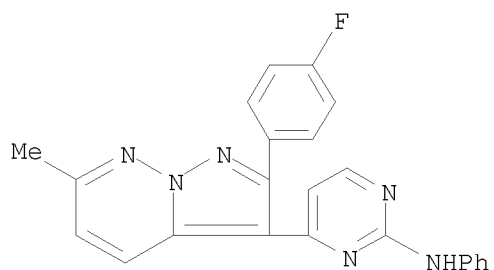


RN 681432-84-8 CAPLUS

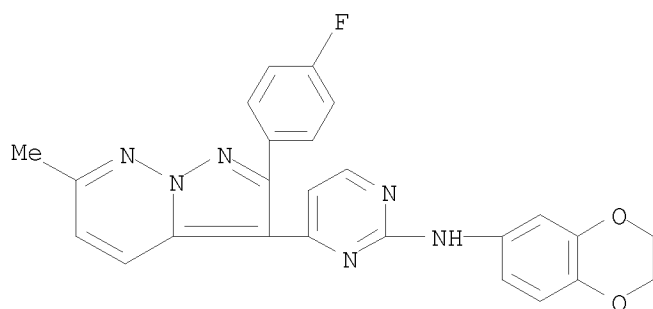
CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[6-methyl-2-[3-(trifluoromethyl)phenyl]pyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



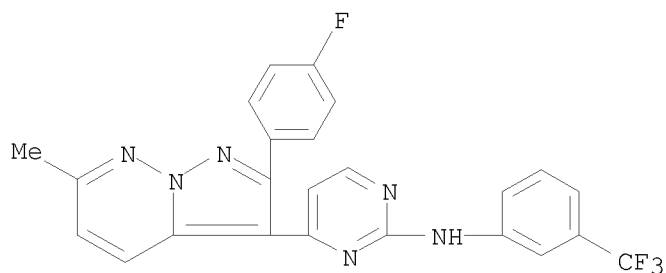
RN 681432-85-9 CAPLUS
 CN 2-Pyrimidinamine, 4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-phenyl- (CA INDEX NAME)



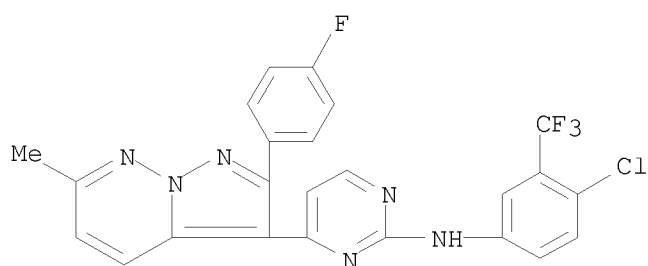
RN 681432-88-2 CAPLUS
 CN 2-Pyrimidinamine, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



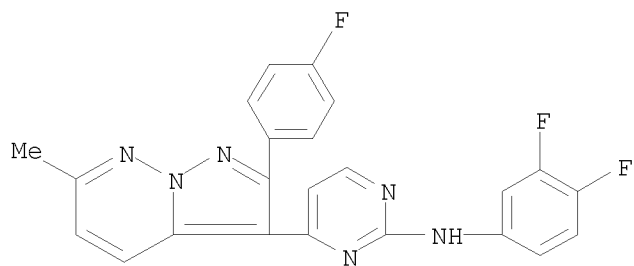
RN 681432-89-3 CAPLUS
 CN 2-Pyrimidinamine, 4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]-N-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 681432-90-6 CAPLUS
 CN 2-Pyrimidinamine, N-[4-chloro-3-(trifluoromethyl)phenyl]-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



RN 681432-91-7 CAPLUS
 CN 2-Pyrimidinamine, N-(3,4-difluorophenyl)-4-[2-(4-fluorophenyl)-6-methylpyrazolo[1,5-b]pyridazin-3-yl]- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log hold		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	36.06	214.63
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-4.80	-4.80

SESSION WILL BE HELD FOR 120 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 10:49:00 ON 11 MAR 2008

Connecting via Winsock to STN